Electronic Supporting Information

Aromatic foldamers as scaffolds for metal second coordination sphere design

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1. Methods for NMR, Infrared Spectroscopy and X-Ray Crystallography

Nuclear Magnetic Resonance. NMR spectra were recorded on 3 different NMR spectrometers: (1) an Avance II NMR spectrometer (Bruker BioSpin) with a vertical 7,05T standard-bore/ultrashield magnet operating at 300 MHz for ^{1}H observation and 75 MHz for ^{13}C observation by means of a 5mm BBFO BB-^{19}F/^{1}H probe with Z-gradients capabilities; (2) an Avance III HD NMR spectrometer (Bruker BioSpin) with a vertical 9.39T standard-bore/ultrashield magnet operating at 400 MHz for ^{1}H observation and 100 MHz for ^{13}C observation by means of a 5mm "Smart Probe" BBFO BB-^{19}F/^{1}H with Z-gradients. (3) an Avance III NMR spectrometer (Bruker BioSpin) with a vertical 16.45T standard-bore/ultrashield magnet operating at 700 MHz for ^{1}H observation and 176 MHz for ^{13}C observation by means of a 5mm BBO ^{1}H-^{19}F/BB probe with Z-or a 5mm TXI ^{1}H/^{13}C/^{15}N probe with Z-gradients capabilities Each probe is connected to a Bruker Cooling Unit II. Chemical shifts are reported in parts per million (ppm, δ) and calibrated against residual ^{1}H and ^{13}C solvent signals. ^{1}H NMR splitting patterns with observed first-order coupling are designated as singlet (s), doublet (d), triplet (t), or multiplet (m). Coupling constants (*J*) are reported in hertz. Data processing was performed with TopSpin 3.2 software.

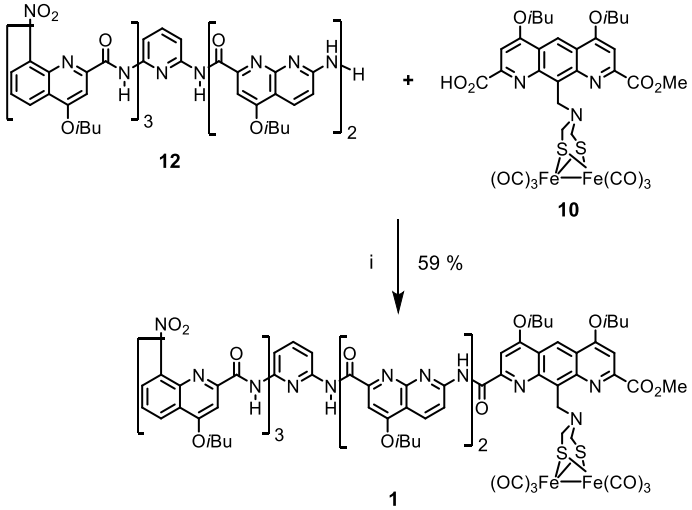
Infrared spectroscopy. Infrared spectra were recorded on a Bruker IFS 55 spectrometer in CaF2 solution cell with a 0.1 mm path length from Specac (omni-cell).

X-Ray Crystallography. The data for crystal structures of compounds **1**, **2** and **3** have been collected at the European Synchrotron Radiation Facility (BM30A beamline). The data were processed using the XDS package.[1] The data for crystal structures of compounds **4** and **5** have been collected at the European Institute for Chemistry and Biology X-ray facility (UMS 3033) on a Rigaku FRX rotating anode at the CuKα wavelength. The system features a micro-focus x-ray source with the hybrid DECTRIS PILATUS 200K detector combined with the partial chi goniometer and the osmic® varimax multilayer optics. The system is driven and the data processed by the CrystalClear suite. The unit cell determinations have been performed using a combination of Fast Fourier and Difference Vector techniques. All the structures have been solved by direct methods with SHELXD or SHELXT and refined by full-matrix least-squares methods using SHELXL.[2] The Coot software[3] was used for modelling. Owing to the size of the molecules, and the thorough task of controlling bond angles and bond lengths, geometric restraints, generated with program PRODRG[4], were applied to each model. It has to be noticed that all the crystals described below contain a large percentage of disordered solvent molecules and very few of them could be modeled in the Fourier difference density maps. Therefore, the SQUEEZE procedure[5] implemented in PLATON[6] was used for all structures in order to treat the regions with highly disordered solvent molecules (mainly chloroform, water, methanol, chlorobenzene or *n*-hexane molecules). Every time where solvent or side chain disorder could be modeled with partial occupancy, it was done so. SHELXL SIMU, DELU or RIGU restraints were used in the refinement strategy, when needed, as listed in the cif files. Hydrogen atoms were positioned theoretically on riding positions using AFIX command. The final cif files were checked using IUCR's checkcif algorithm. Due to the characteristics of the crystals mentioned above (small size, large volume fractions of disordered solvent molecules, side chains disorder, weak diffraction intensity, incompleteness of the data and moderate resolution), a number of A-level and B-level alerts remain in the check cif file.

2. Materials and Methods for chemical synthesis

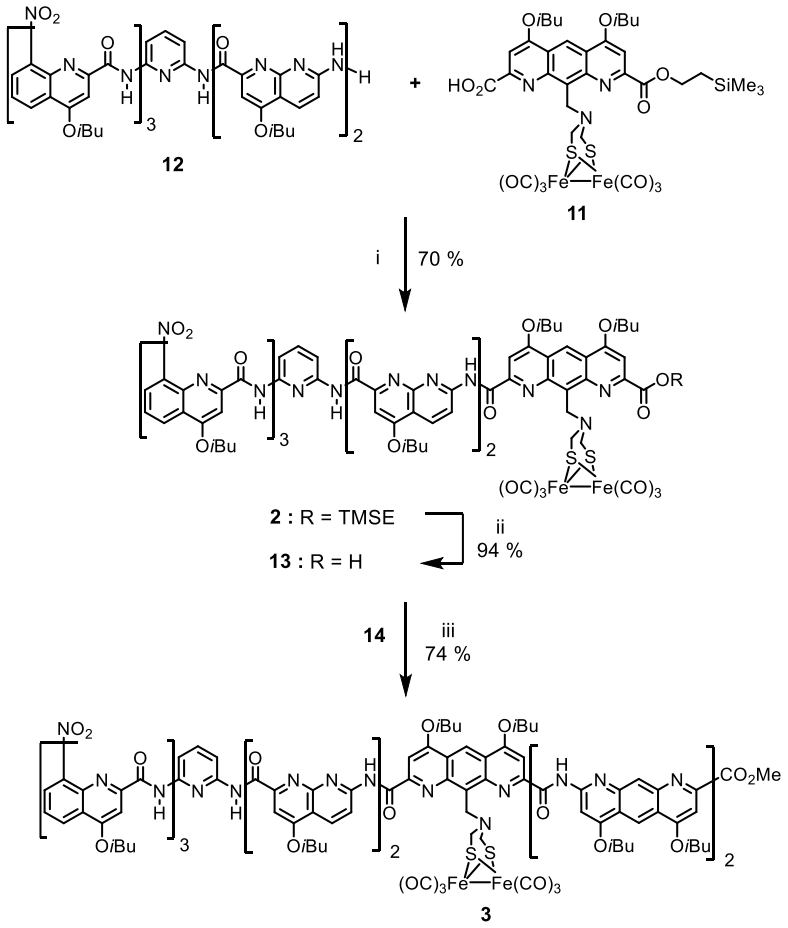
All reactions were carried out under a dry nitrogen atmosphere. Commercial reagents were purchased from Sigma-Aldrich, Alfa-Aesar or TCI and were used without further purification unless otherwise specified. Tetrahydrofurane (THF) dichloromethane (CH_2Cl_2) and toluene were dried over alumina columns; chloroform ($CHCl_3$) and diisopropylethylamine (DIEA) were distilled over calcium hydride (CaH_2) prior to use. Reactions were monitored by thin layer chromatography (TLC) on Merck silica gel 60-F254 plates and observed under UV light. Column chromatography purifications were carried out on Merck GEDURAN Si60 (40-63 µm). Gel permeation chromatography was performed on an LC-9130G NEXT (Japan Analytical Industry Co., Ltd.) setup equipped with two preparative columns (Inner diameter of 20mm and length of 600mm): a JAIGEL 2.5H and a JAIGEL 3H. Column temperatures were regulated at 37 °C in an oven. A mixture of chloroform (HPLC grade, ethanol stabilized) and trimethylamine (0.5% vol/vol) was used for the separations. ESI mass spectra were obtained from the Mass Spectrometry Laboratory at the European Institute of Chemistry and Biology (UMS 3033 - IECB), Pessac, France.

2.1 Synthesis of oligomer 1



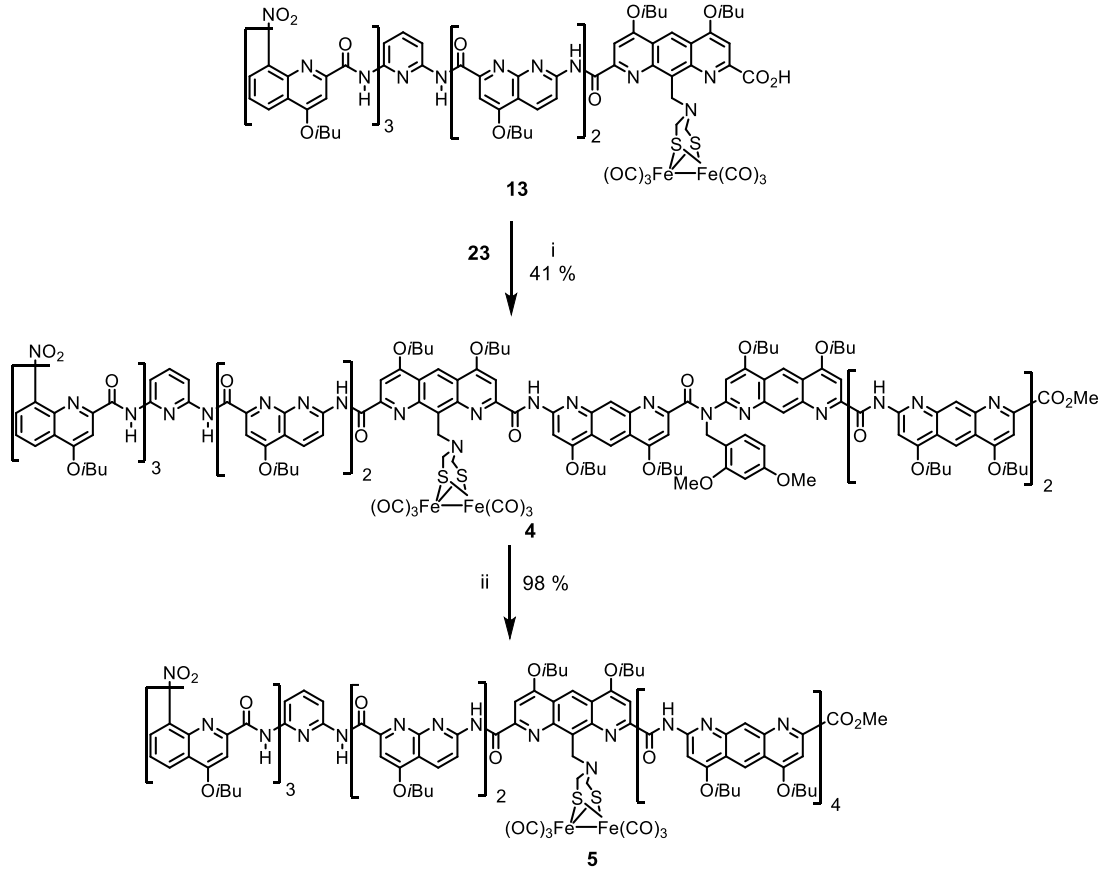
Scheme S1. i) PyBOP, DIEA, $CHCl_3$.

2.2 Synthesis of oligomers 2, 13 and 3



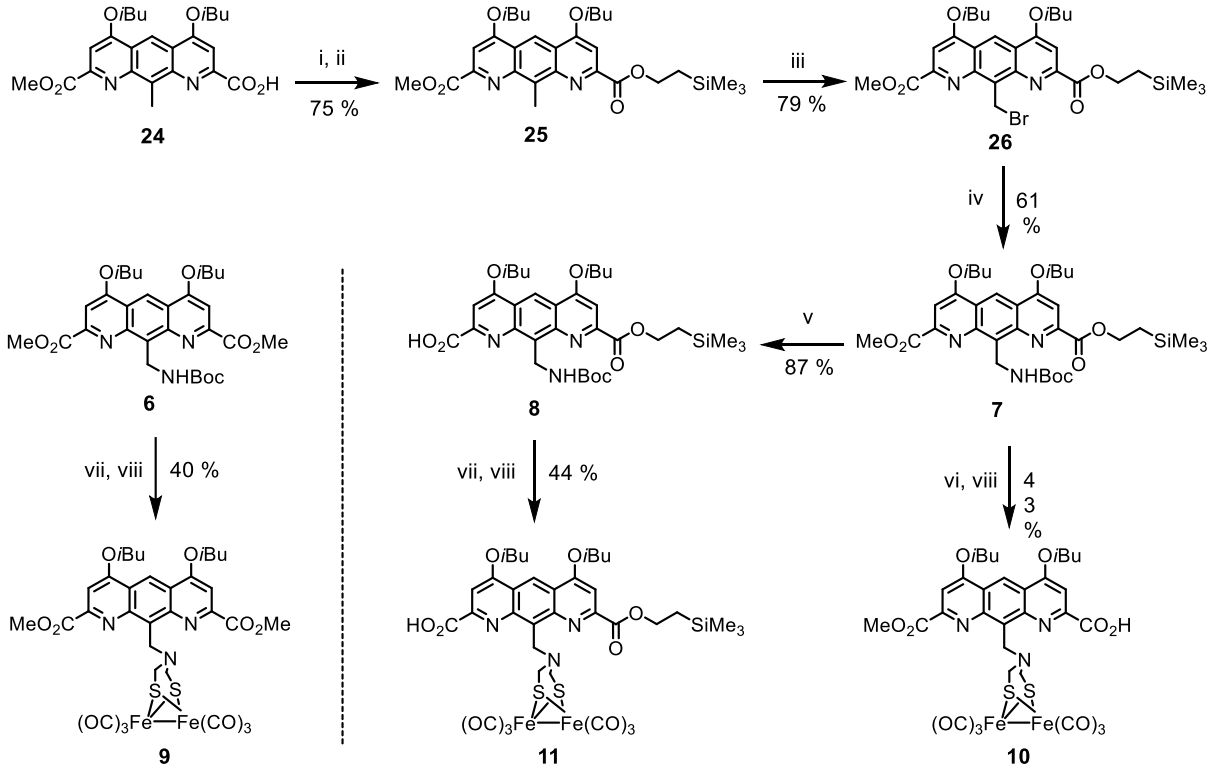
Scheme S2. i) PyBOP, DIEA, CH_2Cl_2, ii) TFA, CH_2Cl_2, iii) PyBOP, DIEA, $CHCl_3$.

2.3 Synthesis of oligomers 4 and 5



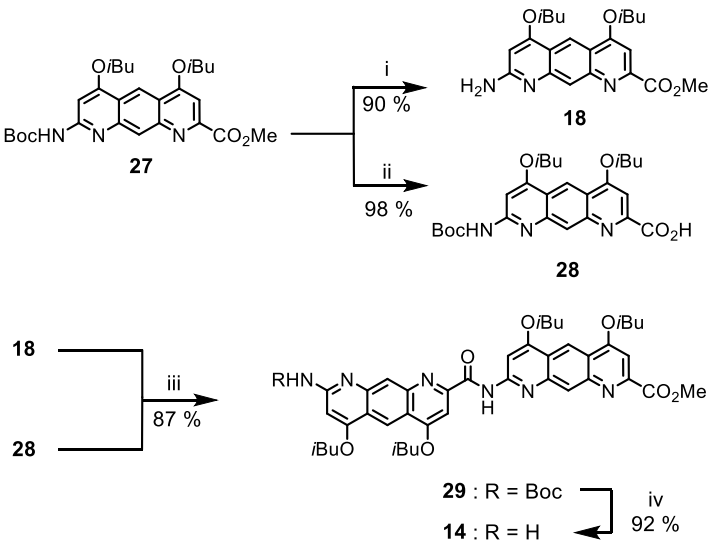
Scheme S3. i) PyBOP, DIEA, $CHCl_3$, ii) TFA, CH_2Cl_2.

2.4 Synthesis of oligomers 9, 10 and 11



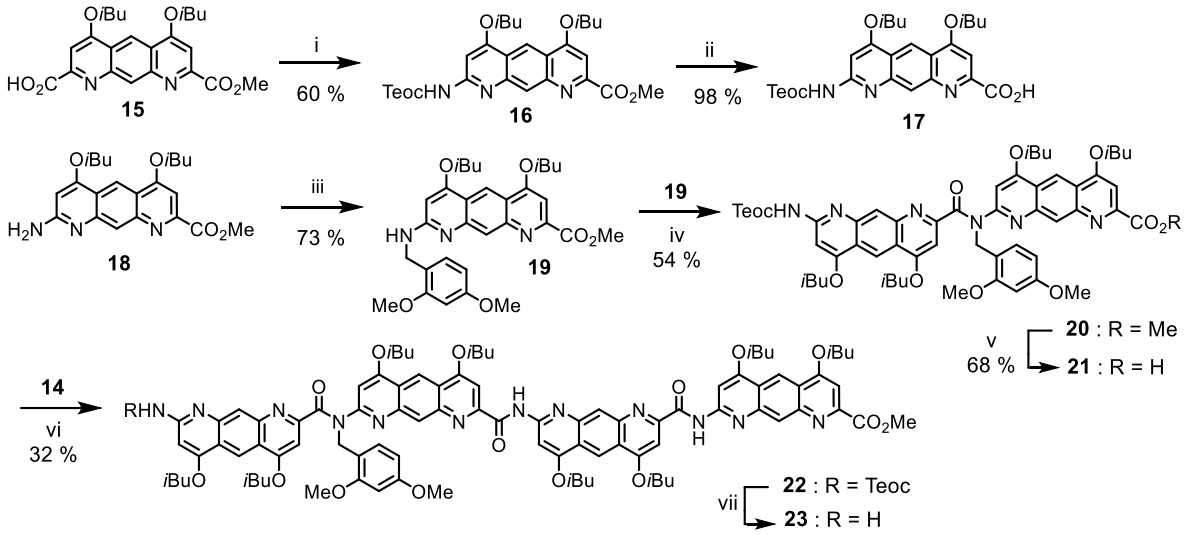
Scheme S4. i) $(COCl)_2$, CH_2Cl_2, ii) TMSEOH, CH_2Cl_2, iii) NBS benzoyl peroxide, benzene, 65°C iv) $KNBoc_2$, DMF, 50°C, v) LiI, EtOAc, dark, 80°C, vi) TFA, CH_2Cl_2, vii) HCl 4M, dioxane, viii) $Fe_2(SH)_2CO_6$, formalin, THF.

2.5 Synthesis of dimer 14



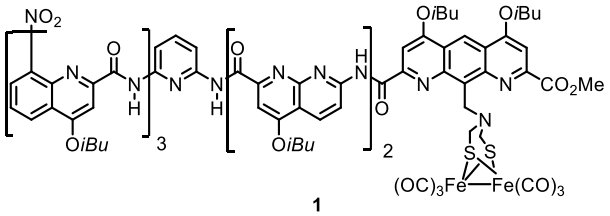
Scheme S5. i) TFA, CH_2Cl_2, ii) $LiOH.H_2O$, THF/MeOH/H_2O, iii) PyBOP, DIEA, $CHCl_3$, iv) TFA, CH_2Cl_2.

2.6 Synthesis of tetramer 23



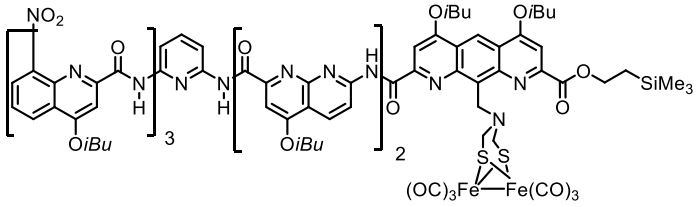
Scheme S6. i) DPPA, DIEA, TMSEOH, toluene, 100°C, ii) $LiOH.H_2O$, THF, MeOH and H_2O, room temperature, iii) 2,4-dimethoxybenzaldehyde, $NaBH(OAc)_3$, DCE, 40°C, iv) PyBOP, DIEA, CH_2Cl_2, room temperature, v) LiI, EtOAc, dark, 80°C, vi) PyBOP, DIEA, $CHCl_3$, room temperature, vii) TBAF, succinic acid, THF, DMF, room temperature.

2.7 Experimental procedures



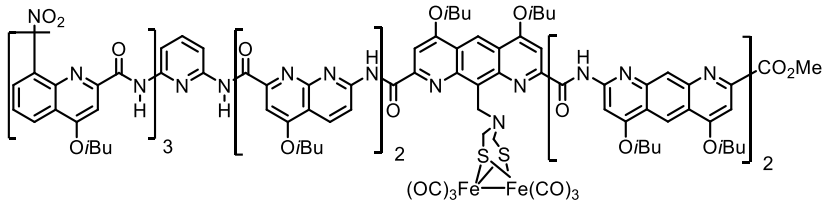
Oligomer 1. Hexamer amine **12**[7] (50 mg, 37 µmol), monomer complex **10** (33 mg, 40 µmol) and PyBOP (38 mg, 73 µmol) were dissolved in dry chloroform (1 mL). Then, DIEA (12 µL, 70 µmol) was added and the reaction mixture was let to stir at room temperature. After 12 hours, the reaction mixture was diluted with dichloromethane and washed with an aqueous saturated solution of NH_4Cl, distilled water and brine. Then, the organic layer was dried over $MgSO_4$, filtered and solvents were removed under reduced pressure. The solid residue was purified by flash chromatography (SiO_2) using cyclohexane:EtOAc (3:1 vol/vol) as eluent to give **1** (47 mg, 59 %) as a red solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ ppm = 11.92 (s, 1H), 11.55 (s, 1H), 11.46 (s, 1H), 11.13 (s, 1H), 10.37 (s, 1H), 9.78 (s, 1H), 8.98 (d, *J* = 9.0 Hz, 1H), 8.91 (s, 1H), 8.87 (d, *J* = 9.0 Hz, 1H), 8.83 (d, *J* = 1.5 Hz, 1H), 8.80 (d, *J* = 1.5 Hz, 1H), 8.46 – 8.40 (m, 2H), 8.29 (d, *J* = 7.5 Hz, 1H), 8.18 (d, *J* = 7.8 Hz, 1H), 7.87 (s, 1H), 7.86 – 7.84 (m, 3H), 7.80 (d, *J* = 7.9 Hz, 1H), 7.75 (s, 1H), 7.72 (d, *J* = 7.7 Hz, 1H), 7.24 (s, 2H), 7.14 (s, 1H), 7.05 (s, 1H), 7.02 (s, 1H), 6.59 (t, *J* = 8.0 Hz, 1H), 6.48 (s, 1H), 6.32 (t, *J* = 8.0 Hz, 1H), 5.05 (d, *J* = 13.6 Hz, 1H), 4.45 (d, *J* = 13.7 Hz, 1H), 4.35 – 4.24 (m, *J* = 15.9, 8.6 Hz, 4H), 4.21 (d, *J* = 6.4 Hz, 3H), 4.19 – 4.12 (m, *J* = 7.1 Hz,

1H), 4.08 – 3.93 (m, 3H), 3.87 – 3.80 (m, 1H), 3.62 (s, 3H), 3.56 (s, 1H), 3.49 – 3.43 (m, 1H), 3.33 – 3.24 (m, 2H), 2.51 – 2.25 (m, 6H), 1.30 (d, *J* = 6.7 Hz, 6H), 1.27 – 1.21 (m, 24H), 0.78 (d, *J* = 6.2 Hz, 3H), 0.52 (d, *J* = 6.5 Hz, 3H). ^{13}C NMR (176 MHz, $CDCl_3$) δ ppm = 207.84, 166.07, 164.58, 164.12, 164.02, 164.00, 163.66, 163.27, 163.05, 162.99, 162.96, 162.64, 161.89, 161.59, 160.74, 154.91, 154.61, 154.58, 153.70, 153.53, 152.66, 151.63, 150.80, 150.15, 149.00, 148.95, 147.15, 145.09, 144.82, 143.74, 139.97, 139.05, 138.20, 135.85, 134.58, 134.43, 134.37, 134.28, 129.86, 128.25, 126.29, 126.12, 125.82, 124.14, 123.55, 122.78, 121.73, 121.31, 120.86, 118.03, 117.12, 115.77, 115.53, 115.50, 115.40, 115.00, 114.89, 114.38, 110.13, 108.46, 101.20, 99.31, 98.57, 98.51, 98.24, 96.92, 96.56, 76.05, 75.89, 75.61, 75.56, 75.40, 75.27, 74.94, 53.45, 53.08, 52.07, 45.95, 29.83, 28.48, 28.40, 28.33, 27.92, 19.64, 19.46, 19.35, 18.57. HRMS (ESI$^+$): *m/z* calcd for $C_{189}H_{196}Fe_2N_{30}O_{35}S_2$ $[M+2H]^{2+}$ 2157.5625 found 2157.5688. IR (cm^{-1}, CH_2Cl_2): $\nu(CO)_{complex}$, 2071, 2033, 1993.



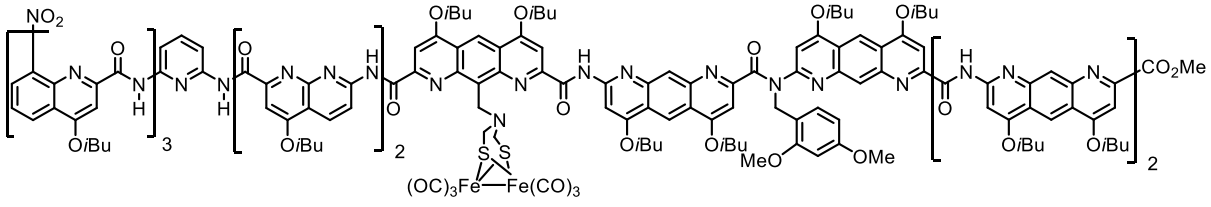
2

Oligomer 2. Amine hexamer **12** (120 mg, 89 µmol), diazaanthracene metal complex **11** (105 mg, 0.115 mmol) and PyBOP (140 mg, 0.27 mmol) were dissolved in dry dichloromethane (2 mL). Then, DIEA (50 µL, 0.27 mmol) was added and the reaction mixture was let to stir at room temperature. After 5 hours, the reaction mixture was diluted with dichloromethane, washed with a saturated aqueous solution of NH_4Cl, distilled water and brine. Then, the organic layer was dried over $MgSO_4$, filtered and the solvent was removed under reduced pressure. The solid residue was purified by flash chromatography (SiO_2) using cyclohexane:EtOAc (3:1 vol/vol) as eluent to give **2** (140 mg, 70 %) as a red solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ ppm = 11.93 (s, 1H), 11.61 (s, 1H), 11.51 (s, 1H), 11.18 (s, 1H), 10.43 (s, 1H), 9.82 (s, 1H), 8.96 (d, *J* = 9.0 Hz, 1H), 8.87 (s, 1H), 8.85 – 8.78 (m, *J* = 9.1, 4.2 Hz, 3H), 8.43 (dd, *J* = 12.9, 4.9 Hz, 2H), 8.30 (d, *J* = 7.7 Hz, 1H), 8.26 (d, *J* = 7.7 Hz, 1H), 7.85 (d, *J* = 2.1 Hz, 3H), 7.78 (t, *J* = 7.9 Hz, 2H), 7.73 – 7.67 (m, *J* = 3.8 Hz, 2H), 7.23 – 7.12 (m, *J* = 7.6 Hz, 3H), 7.04 (dd, *J* = 14.2, 8.3 Hz, 2H), 6.66 (t, *J* = 8.0 Hz, 1H), 6.40 (s, 1H), 6.34 (t, *J* = 8.0 Hz, 1H), 4.78 (dd, *J* = 165.5, 13.5 Hz, 2H), 4.36 – 4.25 (m, *J* = 5.9 Hz, 4H), 4.21 (d, *J* = 6.5 Hz, 4H), 4.07 (d, *J* = 6.3 Hz, 1H), 3.98 (d, *J* = 6.5 Hz, 2H), 3.90 – 3.72 (m, *J* = 13.9 Hz, 3H), 3.61 (s, 1H), 3.56 (s, 3H), 3.31 (d, *J* = 6.1 Hz, 2H), 2.54 – 2.20 (m, 7H), 1.40 – 1.08 (m, 38H), 0.80 (d, *J* = 6.3 Hz, 3H), 0.55 (d, *J* = 6.3 Hz, 3H), -0.10 (s, 9H). ^{13}C NMR (75 MHz, $CDCl_3$) δ ppm = 207.89, 165.67, 164.55, 164.00, 163.97, 163.87, 163.65, 163.10, 163.02, 162.91, 162.83, 162.55, 161.79, 161.46, 160.58, 154.86, 154.80, 154.53, 154.46, 153.66, 153.29, 152.62, 151.47, 150.74, 150.16, 149.69, 149.11, 147.04, 145.03, 144.71, 143.67, 139.87, 139.04, 139.02, 138.09, 135.47, 134.56, 134.30, 128.17, 126.32, 126.05, 125.79, 124.06, 123.48, 122.79, 121.49, 121.15, 120.76, 118.00, 117.06, 115.74, 115.46, 115.35, 114.93, 114.83, 114.24, 109.91, 108.41, 101.08, 99.36, 98.54, 98.35, 98.12, 96.76, 96.40, 75.99, 75.83, 75.58, 75.51, 75.41, 75.27, 74.85, 64.47, 53.38, 51.84, 28.43, 28.36, 28.31, 28.28, 27.89, 19.41, 19.33, 19.29, 18.59, 17.36, -1.60. HRMS (ESI$^+$): *m/z* calcd for $C_{109}H_{113}Fe_2N_{18}O_{23}S_2Si$ $[M+H]^+$ 2243.6176 found 2243.6208. IR (cm^{-1}, CH_2Cl_2): $\nu(CO)_{complex}$, 2071, 2033, 1993.



3

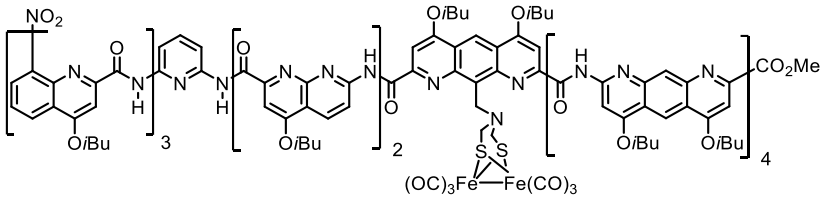
Oligomer 3. Heptamer complex acid **13** (50 mg, 23 µmol), dimer amine **14** (26 mg, 34 µmol) and PyBOP (36 mg, 69 µmol) were dissolved in dry chloroform (1 mL). Then, DIEA (22 µL, 69 µmol) was added and the reaction mixture was let to stir at room temperature. After 12 hours, the reaction mixture was diluted with dichloromethane and washed with an aqueous saturated solution of NH_4Cl, distilled water and brine. Then, the organic layer was dried over Na_2SO_4, filtered and solvents were removed under reduced pressure. The solid residue was purified by flash chromatography (SiO_2) using dichloromethane:acetone (95:5 vol/vol) as eluent to give **3** (50 mg, 74 %) as a red solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ ppm = 11.71 (s, 1H), 11.36 (s, 2H), 11.14 (s, 1H), 10.83 (s, 1H), 10.79 (s, 1H), 10.09 (s, 1H), 9.43 (s, 1H), 9.21 (s, 1H), 9.17 (d, *J* = 9.0 Hz, 1H), 8.95 (s, 1H), 8.91 (s, 1H), 8.89 (d, *J* = 9.0 Hz, 1H), 8.25 (dd, *J* = 7.9, 1.7 Hz, 1H), 8.16 (s, 1H), 8.00 (d, *J* = 7.3 Hz, 2H), 7.97 – 7.89 (m, *J* = 8.5, 4.3 Hz, 5H), 7.80 (s, 2H), 7.65 (s, 1H), 7.56 (s, 1H), 7.44 – 7.38 (m, 2H), 7.24 – 7.21 (m, 2H), 7.17 (t, *J* = 7.7 Hz, 1H), 7.00 (d, *J* = 7.8 Hz, 1H), 6.86 (d, *J* = 8.2 Hz, 1H), 6.81 (s, 1H), 6.77 (d, *J* = 8.2 Hz, 1H), 6.66 (s, 1H), 6.33 (t, *J* = 7.9 Hz, 1H), 6.21 – 6.12 (m, 2H), 5.85 (t, *J* = 8.0 Hz, 1H), 5.23 (d, *J* = 12.6 Hz, 1H), 4.54 (d, *J* = 12.5 Hz, 1H), 4.46 – 4.23 (m, 10H), 4.23 – 4.07 (m, 6H), 4.02 (s, 3H), 3.97 – 3.88 (m, 1H), 3.84 – 3.62 (m, 7H), 3.19 – 3.03 (m, 2H), 2.56 – 2.33 (m, 10H), 2.19 – 2.12 (m, 1H), 1.38 – 1.15 (m, 54H), 1.10 – 1.03 (m, 6H), 0.60 (d, *J* = 6.5 Hz, 3H), 0.30 (d, *J* = 6.7 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ ppm = 207.69, 166.78, 164.50, 164.45, 164.28, 164.04, 163.64, 163.42, 163.24, 162.58, 162.31, 162.13, 161.96, 161.58, 161.38, 159.66, 155.48, 155.16, 154.26, 154.15, 153.56, 152.87, 152.60, 152.05, 151.98, 151.07, 150.89, 150.10, 149.00, 147.76, 147.70, 147.45, 147.16, 146.55, 144.92, 144.57, 143.69, 138.80, 138.57, 137.65, 134.38, 134.28, 134.07, 131.93, 128.04, 127.03, 126.63, 125.75, 123.99, 123.27, 122.58, 122.07, 121.87, 121.27, 120.86, 120.07, 119.66, 119.41, 118.23, 116.64, 116.53, 115.84, 115.71, 115.48, 115.35, 114.72, 113.58, 113.43, 108.32, 106.30, 101.67, 98.77, 98.31, 97.63, 96.76, 95.43, 95.31, 93.69, 92.43, 77.36, 75.97, 75.71, 75.52, 75.27, 75.17, 75.08, 53.92, 53.18, 52.60, 19.74, 19.41, 19.33, 19.29, 18.32, 1.13. HRMS (ESI$^+$): *m/z* calcd for $C_{147}H_{150}Fe_2N_{24}O_{29}S_2$ $[M+2H]^{2+}$ 1445.9581 found 1445.9621. IR (cm^{-1}, CH_2Cl_2): ν(CO), 2072, 2034, 1993.



4

Oligomer 4. Tetramer **22** (70 mg, 39 µmol) was dissolved in dry DMF (10 mL). Then, a solution of tetrabutylammonium fluoride 1M in THF (2 mL) and succinic acid (50 mg, 0.4 mmol) was added and the reaction mixture was stirred at room temperature during 4 hours. After dilution with EtOAc, the organic layer was washed with a saturated aqueous solution of NH_4Cl, distilled water, brine then, the organic layer was dried over $MgSO_4$ and filtered. The solvents were removed under reduced pressure to give **23** as a yellow solid that was used directly

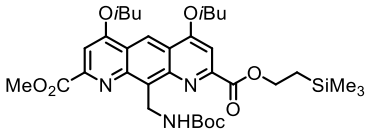
in subsequent reaction without further purification. Heptamer complex acid **13** (70 mg, 33 µmol), tetramer amine (39 µmol) and PyBOP (51 mg, 98 µmol) were dissolved in dry chloroform (2 mL). Then, DIEA (10 µL, 65 µmol) was added and the reaction mixture was stirred at room temperature during 12 hours. The reaction mixture was diluted with dichloromethane and washed with an aqueous saturated solution of NH_4Cl, distilled water and brine. Then, the organic layer was dried over $MgSO_4$, filtered and solvents were removed under reduced pressure. The solid residue was purified by GPC to give **4** (50 mg, 41 %) as a red solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ ppm = 11.76 (s, 1H), 11.40 (s, 2H), 11.32 (s, 1H), 10.99 (s, 1H), 10.90 (s, 1H), 10.48 (s, 1H), 10.24 (s, 1H), 9.54 (s, 1H), 9.16 (s, 1H), 9.09 (s, 1H), 8.94 (s, 2H), 8.79 (d, *J* = 8.4 Hz, 1H), 8.69 (s, 1H), 8.60 (s, 1H), 8.44 (s, 2H), 8.35 – 8.22 (m, 5H), 8.19 (d, *J* = 7.7 Hz, 1H), 8.05 (d, *J* = 7.1 Hz, 2H), 7.74 (s, 3H), 7.71 – 7.66 (m, 1H), 7.63 (s, 1H), 7.58 (s, 1H), 7.48 (s, 1H), 7.39 – 7.31 (m, 2H), 7.23 – 7.08 (m, 5H), 7.06 (d, *J* = 7.7 Hz, 1H), 6.97 (d, *J* = 7.9 Hz, 1H), 6.93 – 6.87 (m, 1H), 6.80 (s, 1H), 6.60 (s, 1H), 6.58 – 6.46 (m, 2H), 6.39 (t, *J* = 8.3 Hz, 1H), 6.20 – 6.01 (m, 2H), 5.48 – 5.17 (m, 3H), 4.72 (d, *J* = 12.6 Hz, 1H), 4.31 – 4.04 (m, 22H), 3.90 (d, *J* = 12.7 Hz, 9H), 3.73 (d, *J* = 4.6 Hz, 3H), 3.59 (s, 3H), 3.48 (s, 3H), 3.17 – 2.96 (m, 3H), 2.65 – 2.01 (m, 15H), 1.34 – 1.14 (m, 72H), 1.09 (d, *J* = 5.0 Hz, 6H), 0.98 (d, *J* = 4.1 Hz, 6H), 0.65 (d, *J* = 5.4 Hz, 3H), 0.37 (d, *J* = 5.6 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ ppm = 207.80, 171.27, 166.24, 163.92, 163.40, 163.29, 162.50, 161.73, 161.27, 159.79, 159.63, 158.14, 157.05, 154.96, 154.69, 154.32, 153.65, 153.32, 152.74, 151.90, 151.54, 150.48, 149.30, 147.69, 147.37, 147.25, 147.04, 146.83, 146.45, 144.49, 143.56, 138.77, 138.18, 137.72, 134.33, 134.11, 133.66, 130.95, 128.06, 126.76, 125.94, 125.61, 123.77, 123.25, 122.49, 121.33, 120.78, 120.49, 119.69, 119.44, 118.99, 118.76, 117.71, 116.66, 116.09, 115.70, 115.25, 114.98, 114.58, 114.35, 113.74, 109.42, 106.89, 103.66, 101.15, 98.98, 98.03, 97.25, 96.10, 95.68, 95.51, 93.82, 92.01, 75.45, 75.14, 75.01, 55.12, 53.88, 53.06, 45.84, 29.73, 28.35, 27.64, 19.25, 18.32, 8.67, 1.05. HRMS (ESI$^+$): *m/z* calcd for $C_{198}H_{206}Fe_2N_{30}O_{37}S_2$ $[M+2H]^{2+}$ 1884.6668 found 1884.6636. IR (cm^{-1}, CH_2Cl_2): $\nu(CO)_{complex}$, 2072, 2030, 1992.



5

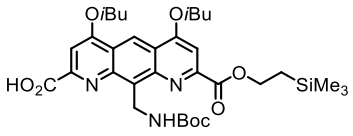
Oligomer 5. Oligomer **4** (25 mg, 0.16 mmol) was dissolved in dry dichloromethane (0.5 mL). Then, TFA (0.5 mL) was added slowly at 0°C and the reaction mixture was stirred at room temperature during 4 hours. The reaction mixture was diluted with dichloromethane and quenched with aqueous saturated $NaHCO_3$ solution. The organic layer was washed with distilled water, brine, then the organic layer was dried over Na_2SO_4 and filtered. The solvent was removed to give **5** (23 mg, 98%) as a red solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ ppm = 11.81 (s, 1H), 11.54 (s, 1H), 11.41 (s, 1H), 11.27 (s, 1H), 11.18 (s, 1H), 10.88 (s, 1H), 10.76 (s, 1H), 10.71 (s, 1H), 10.36 (s, 1H), 9.73 (s, 1H), 9.08 (s, 1H), 9.06 (s, 1H), 8.98 (s, 1H), 8.85 (s, 1H), 8.42 (s, 1H), 8.39 (s, 1H), 8.31 (s, 1H), 8.26 (d, *J* = 7.4 Hz, 1H), 8.16 (d, *J* = 8.3 Hz, 1H), 8.11 (d, *J* = 7.0 Hz, 1H), 8.06 (s, 1H), 8.04 (d, *J* = 7.2 Hz, 1H), 8.02 (s, 1H), 7.98 (s, 1H), 7.88 (s, 1H), 7.83 (d, *J* = 8.3 Hz, 1H), 7.79 (s, 1H), 7.78 (s, 1H), 7.73 (s, 1H), 7.70 (s, 1H), 7.46 (s, 1H), 7.44 (d, *J* = 8.3 Hz, 1H), 7.33 (d, *J* = 8.4 Hz, 1H), 7.19 (s, 1H), 7.18 (s, 2H), 7.14 (s, 1H), 7.13 – 7.11 (m, 2H), 7.09 (t, *J* = 7.2 Hz, 1H), 6.97 (s, 1H), 6.86 (d, *J* = 7.2 Hz, 1H), 6.76 (s, 1H), 6.67 (d, *J* = 7.8 Hz, 1H), 6.52 (d, *J* = 7.6 Hz, 1H), 6.41 – 6.38 (m, 2H), 6.18 (t, *J* = 7.3 Hz, 1H), 6.04 (t, *J* = 7.3 Hz, 1H), 5.89 (t, *J* =

7.4 Hz, 1H), 4.80 (d, *J* = 14.7 Hz, 1H), 4.67 – 4.59 (m, *J* = 15.6 Hz, 4H), 4.44 – 4.35 (m, 6H), 4.26 (t, *J* = 6.7 Hz, 1H), 4.24 – 4.19 (m, 3H), 4.16 (t, *J* = 6.2 Hz, 1H), 4.14 – 4.10 (m, 2H), 4.08 (t, *J* = 7.0 Hz, 1H), 3.99 (t, *J* = 6.1 Hz, 1H), 3.95 – 3.92 (m, 2H), 3.90 – 3.89 (m, 2H), 3.83 (t, *J* = 6.3 Hz, 1H), 3.78 – 3.68 (m, 10H), 3.46 (t, *J* = 7.4 Hz, 1H), 2.84 – 2.81 (m, 1H), 2.52 – 2.42 (m, 8H), 2.39 – 2.20 (m, 7H), 2.16 – 2.11 (m, *J* = 6.8 Hz, 1H), 1.35 – 1.18 (m, 69H), 1.13 (d, *J* = 6.6 Hz, 3H), 1.12 – 1.08 (m, 12H), 0.49 (d, *J* = 6.9 Hz, 3H), 0.26 (d, *J* = 6.6 Hz, 3H). ^{13}C NMR (176 MHz, $CDCl_3$) δ ppm = 208.54, 166.58, 164.30, 164.17, 164.11, 163.88, 163.71, 163.54, 163.39, 163.25, 163.11, 163.01, 162.97, 162.65, 162.55, 162.47, 162.39, 162.34, 162.15, 161.90, 161.50, 161.15, 160.28, 154.77, 154.40, 154.31, 154.20, 153.36, 153.18, 152.90, 152.56, 152.45, 152.33, 152.26, 151.94, 151.49, 151.40, 151.15, 150.69, 150.24, 149.93, 149.53, 148.30, 147.66, 147.47, 147.06, 147.00, 146.89, 146.79, 146.64, 146.36, 146.19, 144.72, 144.59, 143.74, 138.85, 138.18, 137.22, 134.63, 134.45, 134.13, 131.72, 131.61, 130.91, 127.92, 127.34, 126.61, 126.29, 125.76, 125.53, 123.77, 123.38, 122.61, 121.04, 120.73, 120.57, 120.31, 120.18, 119.82, 119.66, 119.48, 118.84, 117.31, 116.41, 115.65, 115.40, 115.28, 114.47, 113.88, 113.47, 112.86, 108.25, 106.72, 101.22, 99.28, 97.48, 97.00, 96.83, 96.77, 95.83, 95.53, 95.26, 95.10, 94.76, 93.97, 93.86, 92.98, 92.64, 75.33, 75.23, 75.15, 75.08, 74.97, 74.84, 74.63, 55.96, 54.51, 52.85, 29.84, 28.73, 28.65, 28.57, 28.55, 28.49, 28.45, 28.40, 28.33, 28.29, 28.23, 28.12, 27.53, 19.60, 19.57, 19.50, 19.44, 19.42, 19.40, 19.35, 19.29, 19.27, 19.16, 18.33, 1.16. HRMS (ESI$^+$): *m/z* calcd for $C_{189}H_{196}Fe_2N_{30}O_{35}S_2$ $[M+2H]^{2+}$ 1809.6327 found 1809.6343. IR (cm^{-1}, CH_2Cl_2): $\nu(CO)_{complex}$, 2072, 2030, 1992, 1969 (sh).



7

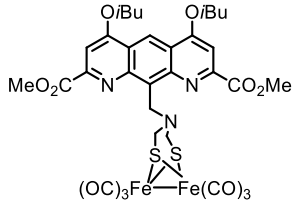
Monomer 7. Bromo-benzyl diazaanthracene **26** (6.5 g, 10.5 mmol) and potassium di-*tert*-butyliminodicarbonate (3.2 g, 12.6 mmol) were dissolved in anhydrous DMF (30 mL). The reaction mixture was stirred for 12 hours at 50°C. After solvent removal on a vacuum line, solid residue and magnesium perchlorate (235 mg, 1.05 mmol) were dissolved in acetonitrile (20 mL) and heated to reflux during 1h. During return to room temperature, a precipitate formed and was filtered, giving **7** as a yellow solid (4.2 g, 61 %). ^{1}H NMR (300 MHz, $CDCl_3$) δ ppm = 9.21 (s, 1H), 7.49 (s, 1H), 7.48 (s, 1H), 5.79 (d, *J* = 6.1 Hz, 2H), 4.61 – 4.53 (m, 2H), 4.13 (d, *J* = 6.4 Hz, 4H), 4.08 (s, 3H), 2.42 – 2.30 (m, 2H), 1.42 (s, 9H), 1.35 – 1.26 (m, 3H), 1.19 (d, *J* = 6.7 Hz, 12H), 0.14 (s, 9H). ^{13}C NMR (75 MHz, $CDCl_3$) δ ppm = 166.45, 165.94, 163.53, 163.46, 156.22, 150.69, 150.41, 145.76, 145.32, 136.51, 121.63, 121.59, 115.83, 98.77, 75.25, 64.67, 53.22, 38.05, 28.65, 28.36, 19.23, 17.58, -1.33. HRMS (ESI$^+$): *m/z* calcd for $C_{34}H_{50}N_3O_8Si$ $[M+H]^+$ 656.3361 found 656.3351.



8

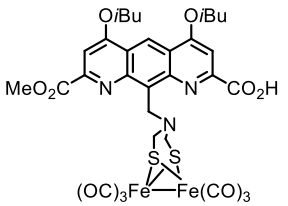
Monomer 8. Methyl ester diazaanthracene **7** (655 mg, 1 mmol) and lithium iodide (160 mg, 1.2 mmol) were dissolved in degassed EtOAc (6 mL). The reaction mixture was stirred at 80°C and protected from light. After 5 hours, the reaction mixture was diluted with EtOAC, washed with an aqueous solution of citric acid (5% wt),

distilled water and brine, then, the organic layer was dried over $MgSO_4$, filtered and solvent was removed. The solid residue was purified by flash chromatography (SiO_2) using dichloromethane:methanol:acetic acid (94:5:1) as eluent. The pure fractions were washed with aqueous saturated solution of $NaHCO_3$, aqueous solution of citric acid (5% wt), water and brine then, the organic layer was dried over Na_2SO_4, filtered and solvents were removed to give **8** as a yellow solid (560 mg, 87%). ^{1}H NMR (300 MHz, $CDCl_3$) δ ppm = 9.24 (s, 1H), 7.59 (s, 1H), 7.48 (s, 1H), 5.76 (d, *J* = 6.6 Hz, 2H), 5.44 (t, *J* = 6.4 Hz, 1H), 4.63 – 4.55 (m, *J* = 9.0, 7.7 Hz, 2H), 4.15 (dd, *J* = 6.3, 5.0 Hz, 4H), 2.43 – 2.31 (m, 2H), 1.42 (s, 9H), 1.31 – 1.24 (m, 2H), 1.19 (dd, *J* = 6.7, 3.4 Hz, 13H), 0.15 (s, 9H). ^{13}C NMR (75 MHz, $CDCl_3$) δ ppm = 165.69, 165.66, 164.21, 163.30, 156.49, 151.41, 149.17, 145.56, 144.01, 136.18, 121.48, 121.40, 116.37, 98.98, 97.28, 79.67, 75.55, 75.29, 64.72, 35.20, 28.56, 28.33, 28.27, 19.21, 19.16, 17.51, -1.29. HRMS (ESI$^+$): *m/z* calcd for $C_{33}H_{48}N_3O_8Si$ $[M+H]^+$ 642.3205 found 642.3205.



9

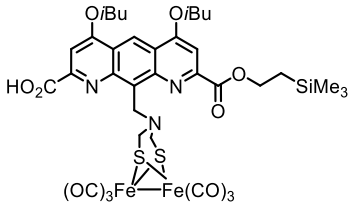
Monomer 9. Boc-protected diazaanthracene **6**[8] (570 mg, 1 mmol) was dissolved in dioxane (8 mL). A solution of HCl 4 M in dioxane (2 mL, 8 mmol) was slowly added at 0°C and the reaction mixture was stirred during 1 hour at room temperature. The solvent was removed under reduced pressure and the resulting ammonium chloride salt was dried under high vacuum. In the meantime, complex $Fe_2S_2(CO)_6$ (344 mg, 1 mmol)[9] was dissolved in dry THF (7.4 mL) and maintained at -78°C. Then, a solution of lithium triethylborohydride 1M in THF (2.2 mL, 2.2 mmol) was added slowly and the reaction mixture was allowed to stir at -78°C. After 30 minutes, TFA (0.18mL, 2.4 mmol) was slowly added and the reaction mixture was allowed to stir at room temperature. After 1 hour, formalin (0.195 mL, 2.6 mmol) was added and the reaction mixture was allowed to stir 2 more hours at room temperature. Then, the last reaction mixture was added to the previous ammonium chloride salt and the whole was stirred during 12 hours at room temperature. Solvent was removed under reduced pressure and the crude was purified by flash chromatography (SiO_2) using cyclohexane:EtOAc (90/10) as eluent, followed by precipitation in hexane to give **9** as a red solid (340 mg, 40 %). ^{1}H NMR (300 MHz, $CDCl_3$) δ ppm = 9.18 (s, 1H), 7.46 (s, 2H), 5.32 (s, 2H), 4.27 – 4.01 (m, 14H), 2.44 – 2.26 (m, 2H), 1.18 (d, *J* = 6.3 Hz, 12H). ^{13}C NMR (75 MHz, $CDCl_3$) δ ppm = 208.34, 166.36, 163.59, 150.53, 145.68, 136.78, 121.88, 116.19, 98.92, 75.39, 53.38, 53.30, 49.82, 28.40, 19.28. HRMS (ESI$^+$): *m/z* calcd for $C_{33}H_{34}Fe_2N_3O_{12}S_2$ $[M+H]^+$ 840.0277 found 840.0296. IR (cm^{-1}, CH_2Cl_2): $\nu(CO)_{complex}$, 2070, 2031, 1993.



10

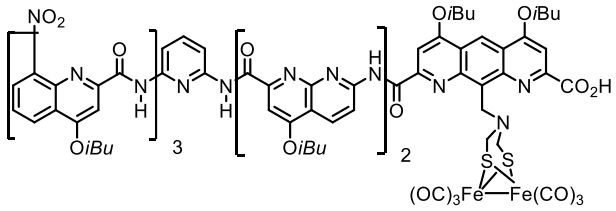
Monomer 10. Boc-protected diazaanthracene **7** (400 mg, 0.61 mmol) was dissolved in dry dichloromethane (3 mL) then, TFA (3 mL) was slowly added at 0°C and the reaction mixture was let to stir at room temperature. After

2 hours, toluene was added and the solvents were removed by rotary evaporation. The resulting ammonium TFA salt diazaanthracene was dried under high vacuum. In the meantime, complex $Fe_2S_2(CO)_6$ (210 mg, 0.61 mmol) was dissolved in dry THF (4.4 mL) and maintained at -78°C. Then, a solution of lithium triethylborohydride 1M in THF (1.3 mL, 1.3 mmol) was added slowly and the reaction mixture was allowed to stir at -78°C. After 30 minutes, TFA (0.11 mL, 1.5 mmol) was slowly added and the reaction mixture was allowed to stir at room temperature. After 1 hour, formalin (0.120 mL, 1.6 mmol) was added and the reaction mixture was allowed to stir 2 more hours at room temperature. Then, the last reaction mixture was added to the previous ammonium TFA salt diazaanthracene and the whole was stirred during 12 hours at room temperature. Solvent was removed under reduced pressure and the residue was purified by flash chromatography (SiO_2) using dichloromethane:methanol (98/2) as eluent, followed by precipitation in hexane to give **10** as a red solid (225 mg, 43 %). ^{1}H NMR (300 MHz, $CDCl_3$) δ ppm = 9.27 (s, 1H), 7.59 (s, 1H), 7.51 (s, 1H), 5.28 (s, 2H), 4.18 (d, *J* = 6.4 Hz, 2H), 4.14 (d, *J* = 6.4 Hz, 2H), 4.10 (s, 3H), 3.98 (s, 4H), 2.44 – 2.30 (m, 2H), 1.19 (d, *J* = 6.1 Hz, 12H). ^{13}C NMR (75 MHz, $CDCl_3$) δ ppm = 207.84, 165.89, 165.06, 163.48, 150.89, 146.06, 134.58, 121.89, 121.62, 117.04, 99.32, 75.83, 75.41, 53.25, 53.10, 49.47, 28.24, 19.09. HRMS (ESI$^+$): *m/z* calcd for $C_{32}H_{32}Fe_2N_3O_{12}S_2$ $[M+H]^+$ 826.0120 found 826.0147. IR (cm^{-1}, CH_2Cl_2): $\nu(CO)_{complex}$, 2072, 2033, 1995.



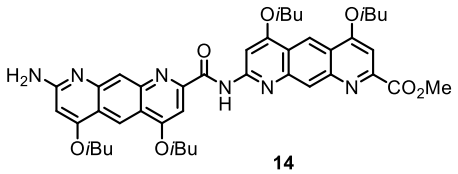
11

Monomer 11. Boc-protected diazaanthracene **8** (640 mg, 1 mmol) was dissolved in dioxane (8 mL). A solution of HCl 4M in dioxane (2 mL, 8 mmol) was slowly added at 0°C and the reaction mixture was stirred during 1 hour at room temperature. The solvent was removed under reduced pressure and the resulting ammonium chloride salt diazaanthracene was dried under high vacuum. In the meantime, complex $Fe_2S_2(CO)_6$ (344 mg, 1 mmol) was dissolved in dry THF (7.4 mL) and maintained at -78°C. Then, a solution of lithium triethylborohydride 1M in THF (2.2 mL, 2.2 mmol) was added slowly and the reaction mixture was allowed to stir at -78°C. After 30 minutes, TFA (0.18 mL, 2.4 mmol) was slowly added and the reaction mixture was allowed to stir at room temperature. After 1 hour, formalin (0.195 mL, 2.6 mmol) was added and the reaction mixture was allowed to stir 2 more hours at room temperature. Then, the last reaction mixture was added to the previous ammonium chloride salt diazaanthracene and the whole was stirred during 12 hours at room temperature. The solvent was removed under reduced pressure and the crude was purified by precipitation in diethyl ether to give **11** as a red solid (400 mg, 44%).^{1}H NMR (300 MHz, $CDCl_3$) δ ppm = 9.26 (s, 1H), 7.58 (s, 1H), 7.50 (s, 1H), 5.26 (s, 2H), 4.60 – 4.53 (m, *J* = 9.5, 7.8 Hz, 2H), 4.18 (d, *J* = 6.3 Hz, 2H), 4.13 (d, *J* = 6.4 Hz, 2H), 3.98 (s, 4H), 2.44 – 2.28 (m, 2H), 1.34 – 1.27 (m, *J* = 9.6, 7.7 Hz, 2H), 1.19 (dd, *J* = 6.7, 1.8 Hz, 12H), 0.14 (s, 9H). ^{13}C NMR (75 MHz, $CDCl_3$) δ ppm = 207.99, 165.74, 165.21, 164.24, 163.64, 151.59, 149.61, 146.37, 143.97, 134.84, 122.17, 121.78, 117.25, 99.43, 97.02, 75.96, 75.52, 64.93, 53.38, 49.86, 28.39, 19.24, 17.88, -1.30. HRMS (ESI$^+$): *m/z* calcd for $C_{36}H_{42}Fe_2N_3O_{12}S_2Si$ $[M+H]^+$ 912.0672 found 912.0674. IR (cm^{-1}, CH_2Cl_2): $\nu(CO)_{complex}$, 2072, 2033, 1997.



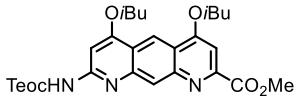
13

Oligomer 13. Oligomer **2** (350 mg, 0.16 mmol) was dissolved in dry dichloromethane (2 mL). Then, TFA (4 mL) was added slowly at 0°C and the reaction mixture was let to stir at room temperature. After 2 hours, the reaction mixture was diluted with dichloromethane and quenched with aqueous saturated $NaHCO_3$ solution. The organic layer was washed with distilled water, brine then, dried over Na_2SO_4 and filtered. The solvent was removed under reduced pressure to give **13** (315 mg, 94 %) as a red solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ ppm = 11.91 (s, 1H), 11.54 (s, 1H), 11.39 (s, 1H), 11.27 (s, 1H), 10.18 (s, 1H), 9.74 (s, 1H), 9.12 (s, 1H), 9.00 (d, *J* = 8.9 Hz, 1H), 8.92 – 8.75 (m, 3H), 8.46 (d, *J* = 7.2 Hz, 2H), 8.24 (d, *J* = 7.5 Hz, 1H), 8.10 (d, *J* = 7.7 Hz, 1H), 8.05 (s, 1H), 7.95 – 7.69 (m, 6H), 7.31 (s, 1H), 7.23 (s, 1H), 7.15 (s, 1H), 7.09 (d, *J* = 7.9 Hz, 1H), 7.03 (d, *J* = 8.1 Hz, 1H), 6.65 (s, 1H), 6.53 (t, *J* = 7.6 Hz, 1H), 6.37 (t, *J* = 7.8 Hz, 1H), 4.74 (dd, *J* = 173.3, 11.5 Hz, 2H), 4.40 – 4.14 (m, 8H), 4.03 (d, *J* = 23.3 Hz, 3H), 3.86 (s, 1H), 3.70 (s, 1H), 3.55 (s, 1H), 3.36 (d, *J* = 17.1 Hz, 4H), 2.61 – 2.17 (m, 7H), 1.37 – 1.13 (m, 36H), 0.76 (s, 3H), 0.50 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ ppm = 207.50, 164.63, 164.51, 164.21, 164.11, 164.00, 163.90, 163.79, 163.42, 163.14, 163.09, 162.41, 162.11, 161.59, 160.38, 155.00, 154.94, 154.58, 153.80, 153.68, 152.83, 152.62, 150.67, 149.83, 148.75, 148.45, 147.59, 145.12, 144.91, 143.65, 140.19, 139.04, 138.34, 134.60, 134.44, 133.21, 128.29, 126.47, 126.28, 125.68, 124.13, 123.62, 122.82, 122.07, 121.38, 121.08, 118.10, 117.30, 117.02, 115.81, 115.65, 115.43, 114.99, 114.83, 114.59, 110.26, 109.03, 101.25, 99.44, 98.73, 98.52, 97.52, 97.32, 96.60, 76.05, 75.93, 75.83, 75.75, 75.66, 75.44, 75.13, 53.32, 51.63, 28.48, 28.41, 28.33, 27.95, 19.48, 19.44, 19.37, 19.33, 19.27. HRMS (ESI$^+$): *m/z* calcd for $C_{104}H_{101}Fe_2N_{18}O_{23}S_2$ $[M+H]^+$ 2143.5468 found 2143.5520. IR (cm^{-1}, CH_2Cl_2): $\nu(CO)_{complex}$, 2073, 2035, 1995.



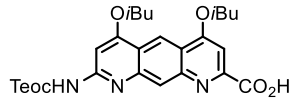
14

Dimer 14. Boc-protected dimer **29** (500 mg, 0.58 mmol) was dissolved in dichloromethane (3 mL). Then, TFA (3 mL) was added slowly at 0°C and the reaction mixture was let to stir at room temperature. After 2 hours, the reaction mixture was diluted with dichloromethane and quenched with aqueous saturated $NaHCO_3$ solution. The organic solvent was removed by rotary evaporation allowing precipitation of the dimer amine in basic aqueous solution. The precipitate was collected by filtration and washed with distilled water on the filter. Then, the solid was dissolved again in dichloromethane then, the organic layer was dried over Na_2SO_4, filtered and solvents were removed under reduced pressure to give **14** as a yellow solid (410 mg, 92 %). ^{1}H NMR (300 MHz, $CDCl_3$) δ ppm = 11.13 (s, 1H), 9.17 (s, 1H), 9.00 (s, 1H), 8.82 (s, 1H), 8.44 (s, 1H), 8.22 (s, 1H), 7.63 (s, 1H), 7.47 (s, 1H), 6.08 (s, 1H), 4.23 – 4.09 (m, 11H), 4.00 (d, *J* = 6.1 Hz, 2H), 2.43 – 2.30 (m, 4H), 1.20 (t, *J* = 7.5 Hz, 24H). HRMS (ESI$^+$): *m/z* calcd for $C_{43}H_{51}N_6O_7$ $[M+H]^+$ 763.3813 found 763.3812.



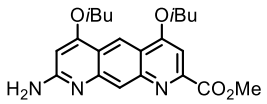
16

Monomer 16. Mono-acid diazaanthracene **15**[8] (3 g, 7 mmol) was dispersed in dry toluene (105 mL) and the mixture was sonicated to obtain a fine slurry. Then, DIEA (2.4 mL, 14 mmol), diphenylphosphoryl azide (3 mL, 14 mmol) and 2-trimethylsilylethanol (6 mL, 42 mmol) were added to the slurry. The reaction mixture was stirred vigorously at 100°C for 3 hours. The solvents were removed under reduced pressure and the residue was dissolved in dichloromethane, washed with a 2M NaOH aqueous solution, distilled water and brine. Then the organic layer was dried over Na_2SO_4, filtered and the solvent was removed under reduced pressure. The residue was purified by flash chromatography (SiO_2) using dichloromethane:acetone (95:5 vol/vol) as eluent to give **16** (2.3 g, 60 %) as a yellow solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ ppm = 9.11 (s, 1H), 8.62 (s, 1H), 7.78 – 7.61 (m, 2H), 7.45 (s, 1H), 4.36 – 4.28 (m, 2H), 4.15 – 4.06 (m, 7H), 2.42 – 2.26 (m, 2H), 1.18 (dd, *J* = 6.7, 4.7 Hz, 12H), 1.13 – 1.05 (m, 2H), 0.09 (s, 9H). ^{13}C NMR (75 MHz, $CDCl_3$) δ ppm = 166.51, 163.61, 154.59, 153.99, 151.05, 148.14, 147.18, 126.20, 120.68, 119.48, 116.80, 98.34, 92.47, 75.16, 75.05, 64.18, 53.44, 28.42, 19.32, 19.28, 17.59, -1.42. HRMS (ESI$^+$): *m/z* calcd for $C_{28}H_{40}N_3O_6Si$ $[M+H]^+$ 542.2680 found 542.2683.



17

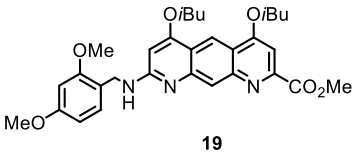
Monomer 17. Methyl ester diazaanthracene **16** (2.3 g, 4.25 mmol) was dissolved in THF (30 mL) then, distilled water (10 mL) and lithium hydroxide monohydrate (360 mg, 8.5 mmol) were added. The reaction mixture was let to stir at room temperature. After 2 hours, the reaction mixture was quenched by addition of citric acid monohydrate (3.57 g, 17 mmol) dissolved in distilled water (30 mL). The organic solvent was removed by rotary evaporation allowing precipitation of the acid diazaanthracene in acidic aqueous solution. The precipitate was collected by filtration and washed with distilled water on the filter. Then, the solid residue was dissolved in dichloromethane, the organic layer was dried over Na_2SO_4, filtered and the solvent was removed under reduced pressure to give **17** as yellow solid (2.1 g, 98 %). ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.01 (s, 1H), 8.86 (s, 1H), 7.78 (s, 1H), 7.63 (s, 1H), 4.35 – 4.27 (m, 2H), 4.21 (d, *J* = 6.1 Hz, 2H), 4.08 (d, *J* = 6.3 Hz, 2H), 2.40 – 2.30 (m, 2H), 1.18 (dd, *J* = 6.6, 4.1 Hz, 12H), 1.11 – 1.04 (m, 2H), 0.06 (s, 9H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.43, 163.69, 163.54, 155.37, 153.86, 152.38, 146.92, 142.82, 121.17, 120.22, 118.38, 117.53, 97.81, 92.60, 76.02, 75.08, 64.25, 28.18, 19.08, 18.97, 17.51, -1.57. HRMS (ESI$^+$): *m/z* calcd for $C_{27}H_{38}N_3O_6Si$ $[M+H]^+$ 528.2524 found 528.2530.



18

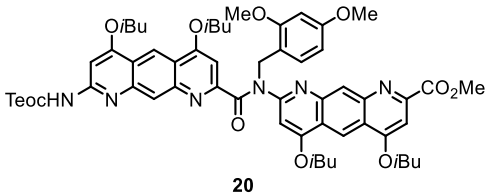
Monomer 18. Boc-protected diazaanthracene **27**[8] (1.8 g, 3.6 mmol) was dissolved in dichloromethane (8 mL). Then, TFA (4 mL) was added slowly at 0°C and the reaction mixture was let to stir at room temperature. After 2 hours, the reaction mixture was diluted with dichloromethane and quenched with aqueous saturated $NaHCO_3$ solution. The organic solvent was removed by rotary evaporation allowing precipitation of the amine diazaanthracene in basic aqueous solution. The precipitate was collected by filtration and washed with distilled water on the filter. Then, the solid residue was dissolved in dichloromethane, the organic layer was dried over

Na_2SO_4, filtered and solvent was removed under reduced pressure to give **18** as a yellow solid (1.3 g, 90 %). ^{1}H NMR (300 MHz, $CDCl_3$) δ ppm = 8.99 (s, 1H), 8.43 (s, 1H), 7.41 (s, 1H), 6.05 (s, 1H), 4.98 (s, 1H), 4.13 – 4.06 (m, 5H), 3.96 (d, *J* = 6.3 Hz, 2H), 2.39 – 2.26 (m, 2H), 1.18 (dd, *J* = 6.7, 2.8 Hz, 12H). ^{13}C NMR (75 MHz, d^6 - DMSO) δ ppm = 165.77, 162.61, 160.55, 150.08, 149.28, 147.91, 121.19, 119.31, 116.14, 115.00, 97.50, 92.33, 74.27, 73.78, 52.64, 27.81, 27.71, 18.82. HRMS (ESI$^+$): *m/z* calcd for $C_{22}H_{28}N_3O_4$ $[M+H]^+$ 398.2074 found 398.2061.



19

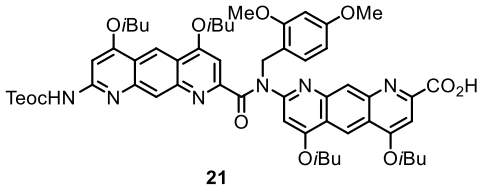
Monomer 19. Amine diazaanthracene **18** (398 mg, 1 mmol) and 2,4-dimethoxybenzaldehyde (498 mg, 3 mmol) were dissolved in 1,2-dichloroethane (5mL) then, sodium triacetoxyborohydride (635 mg, 3 mmol) was added and the reaction mixture was let to stir at 40°C. After 5 days, the reaction mixture was diluted with dichloromethane and quenched with aqueous saturated $NaHCO_3$ solution. The organic layer was washed with distilled water, brine then, dried over $MgSO_4$, filtered and the solvents were removed under reduced pressure. The residue was purified by flash chromatography (SiO_2) using dichloromethane:acetone (8:2 vol/vol) as eluent to give **19** (400 mg, 73 %) as a yellow solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ ppm = 8.91 (s, 1H), 8.45 (s, 1H), 7.41 (d, *J* = 8.2 Hz, 1H), 7.37 (s, 1H), 6.48 (d, *J* = 2.3 Hz, 1H), 6.44 (dd, *J* = 8.2, 2.4 Hz, 1H), 5.96 (s, 1H), 5.30 (s, 1H), 4.68 (d, *J* = 5.5 Hz, 2H), 4.11–4.06 (m, 5H), 3.90 (d, *J* = 6.4 Hz, 2H), 3.86 (s, 3H), 3.79 (s, 3H), 2.39–2.21 (m, 2H), 1.15 (dd, *J* = 8.9, 6.8 Hz, 12H). ^{13}C NMR (75 MHz, $CDCl_3$) δ ppm = 166.68, 163.42, 161.57, 160.29, 158.79, 158.59, 150.15, 149.34, 148.67, 130.97, 123.49, 120.21, 119.65, 117.36, 115.85, 103.87, 98.48, 97.52, 91.21, 74.75, 74.21, 55.36, 55.30, 53.15, 40.72, 28.30, 28.18, 19.15, 19.13. HRMS (ESI$^+$): *m/z* calcd for $C_{31}H_{38}N_3O_6$ $[M+H]^+$ 548.2755 found 548.2755.



20

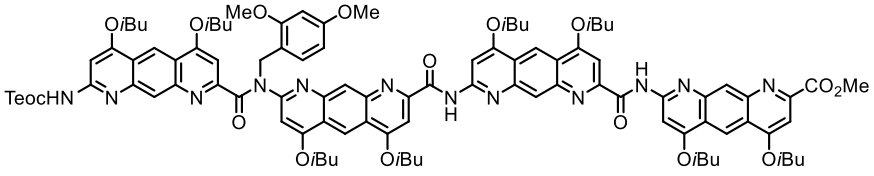
Dimer 20. Secondary amine diazaanthracene **19** (620 mg, 1.14 mmol), acid diazaanthracene **17** (600 mg, 1.14 mmol) and PyBOP (1.18 g, 2.27 mmol) were dissolved in dry dichloromethane (5 mL). Then, DIEA (0.290 mL, 1.7 mmol) was added and the reaction mixture was let to stir at room temperature. After 3 hours, the reaction mixture was diluted with dichloromethane, washed with a saturated aqueous solution of NH_4Cl, distilled water and brine then, the organic layer was dried over $MgSO_4$, filtered and the solvent was removed under reduced pressure. The residue was purified by GPC to give **20** (650 mg, 54 %) as a yellow solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ ppm = 8.96 (s, 2H), 8.44 (s, 1H), 7.95 (s, 1H), 7.66 (d, *J* = 8.4 Hz, 1H), 7.59 (s, 1H), 7.49 (s, 1H), 7.36 (s, 1H), 7.08 (s, 1H), 6.81 (s, 1H), 6.45 (dd, *J* = 8.4, 2.4 Hz, 1H), 6.32 (d, *J* = 2.2 Hz, 1H), 5.46 (s, 2H), 4.31 – 4.22 (m, 2H), 4.11 – 3.93 (m, 9H), 3.82 (d, *J* = 6.4 Hz, 2H), 3.75 (s, 3H), 3.51 (s, 3H), 2.38 – 2.21 (m, 3H), 2.21 – 2.08 (m, 1H), 1.21 – 1.08 (m, 18H), 1.09 – 0.97 (m, 8H), 0.05 (s, 9H). ^{13}C NMR (75 MHz, $CDCl_3$) δ ppm = 170.79, 166.19, 164.15, 163.35, 162.79, 162.45, 160.19, 158.23, 158.11, 157.92, 154.20, 153.98, 150.71, 147.57,

147.42, 146.61, 130.68, 127.41, 123.11, 120.56, 120.07, 119.05, 118.84, 118.09, 116.98, 116.43, 104.23, 98.74, 98.33, 98.20, 97.68, 91.73, 75.09, 75.01, 74.94, 74.80, 64.19, 55.28, 55.15, 53.28, 46.04, 28.22, 28.02, 19.15, 19.12, 19.04, 17.39, -1.58. HRMS (ESI$^+$): *m/z* calcd for $C_{58}H_{73}N_6O_{11}Si$ $[M+H]^+$ 1057.5101 found 1057.5116.



21

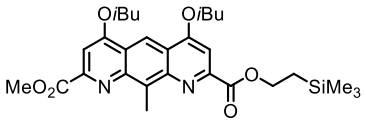
Dimer 21. Diazaanthracene dimer **20** (215 mg, 0.2 mmol) and lithium iodide (136 mg, 1 mmol) were dissolved in degassed EtOAc (5 mL). The reaction mixture was stirred at 80°C and protected from light. After 4 hours, the reaction mixture was let to reach room temperature and the precipitate that formed during the reaction was filtered. The precipitate was dissolved in dichloromethane, washed with an aqueous solution of citric acid (5% wt), distilled water and brine then, the organic layer was dried over Na_2SO_4, filtered and solvent was removed to give **21** as a yellow solid (145 mg, 68 %). ^{1}H NMR (300 MHz, $CDCl_3$) δ ppm = 9.03 (s, 1H), 8.99 (s, 1H), 8.32 (s, 1H), 7.96 (s, 1H), 7.63 (s, 1H), 7.61 (s, 1H), 7.47 (s, 1H), 7.09 (s, 1H), 6.82 (s, 1H), 6.47 (d, *J* = 7.6 Hz, 1H), 6.32 (s, 1H), 5.49 (s, 2H), 4.32 – 4.24 (m, 2H), 4.11 (d, *J* = 6.4 Hz, 2H), 4.08 – 3.98 (m, 4H), 3.81 (d, *J* = 5.7 Hz, 2H), 3.76 (s, 3H), 3.47 (s, 3H), 2.37 – 2.24 (m, 4H), 1.14 (dd, *J* = 6.6, 3.1 Hz, 18H), 1.10 – 0.99 (m, 8H), 0.06 (s, 9H). ^{13}C NMR (75 MHz, $CDCl_3$) δ ppm = 170.74, 165.48, 164.91, 162.81, 162.62, 160.33, 158.71, 158.22, 154.22, 153.62, 151.10, 147.96, 147.09, 144.50, 130.40, 124.62, 120.83, 119.80, 119.40, 118.09, 117.54, 104.36, 99.28, 98.37, 97.19, 91.35, 75.80, 75.18, 74.99, 64.85, 55.41, 55.23, 46.18, 29.78, 28.49, 28.07, 19.18, 19.10, 17.63, -1.44. HRMS (ESI$^+$): *m/z* calcd for $C_{57}H_{71}N_6O_{11}Si$ $[M+H]^+$ 1043.4944 found 1043.4988.



22

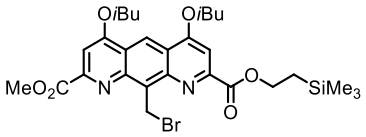
Tetramer 22. Acid dimer **21** (100 mg, 0.096 mmol), amine dimer **14** (95 mg, 0.12 mmol) and PyBOP (150 mg, 0.29 mmol) were dissolved in dry chloroform (2 mL). Then, DIEA (40 µL, 0.23 mmol) was added and the reaction mixture was let to stir at room temperature. After 12 hours, the reaction mixture was diluted with dichloromethane, washed with a saturated aqueous solution of NH_4Cl, distilled water and brine then, the organic layer was dried over $MgSO_4$, filtered and the solvents were removed under reduced pressure. The residue was purified by GPC to give **22** (55 mg, 32 %) as a yellow solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ ppm = 11.10 (s, 1H), 11.01 (s, 1H), 9.08 (d, *J* = 5.8 Hz, 2H), 8.99 (d, *J* = 3.5 Hz, 2H), 8.82 (s, 1H), 8.73 (s, 1H), 8.58 (s, 1H), 8.18 (d, *J* = 6.8 Hz, 2H), 8.08 (s, 1H), 7.69 (d, *J* = 8.5 Hz, 2H), 7.61 (s, 1H), 7.60 (s, 1H), 7.56 (s, 1H), 7.43 (s, 1H), 7.09 (s, 1H), 6.91 (s, 1H), 6.51 (dd, *J* = 8.5, 2.3 Hz, 1H), 6.37 (d, *J* = 2.2 Hz, 1H), 5.57 (s, 2H), 4.30 – 4.23 (m, 2H), 4.19 – 4.04 (m, 15H), 4.01 (d, *J* = 6.4 Hz, 2H), 3.86 – 3.75 (m, 5H), 3.58 (s, 3H), 2.45 – 2.22 (m, 8H), 1.26 – 0.99 (m, 50H), 0.05 (s, 9H). ^{13}C NMR (75 MHz, $CDCl_3$) δ ppm = 170.80, 166.46, 163.86, 163.62, 163.44, 162.83, 162.20, 160.13, 158.26, 157.89, 157.62, 153.64, 151.93, 151.72, 150.92, 148.03, 147.59, 147.40, 147.10, 146.93, 146.75, 130.47, 127.04, 126.82, 125.97, 124.50, 120.86, 120.73, 120.60, 120.20, 119.64, 118.84, 118.48, 116.74, 116.59, 104.21, 98.59,

98.23, 95.63, 93.66, 93.53, 91.57, 75.14, 74.98, 74.85, 64.05, 55.37, 55.24, 53.35, 46.37, 29.71, 28.36, 28.23, 28.01, 19.27, 19.17, 19.05, 17.55, -1.47. HRMS (ESI$^+$): *m/z* calcd for $C_{100}H_{119}N_{12}O_{17}Si$ $[M+H]^+$ 1787.8580 found 1787.8652.



25

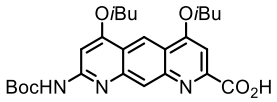
Monomer 25. Monoacid 9-méthyldiazaanthracene **24**[8] (10 g, 21.6 mmol) was dissolved in dry dichloromethane (44 mL). A needle was inserted into the septum to act as a gas vent while oxalyl chloride (5.56 mL, 64.8 mmol) was added slowly to the mixture and the reaction mixture was let to stir at room temperature. After 3 hours, solvent was removed under vacuum and the resulting acyl chloride diazaanthracene was dried under high vacuum. Then, the solid was dissolved in dry dichloromethane (44 mL), 2-trimethylsilylethanol (3.18 mL, 23.8 mmol) was added and the reaction mixture was let to stir at room temperature. After 12 hours, the reaction mixture was quenched with aqueous saturated $NaHCO_3$ solution, the organic layer was washed with water and brine then, dried over $MgSO_4$, filtered and solvent was removed under reduced pressure. The residue was dissolved in dichloromethane then, methanol was added and dichloromethane was slowly removed by rotary evaporation allowing precipitation of the diazaanthracene. The precipitate was filtered, washed with cold methanol on the filter and dried under vacuum to give **25** (8.84 g, 75%) as a yellow solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ ppm = 9.17 (s, 1H), 7.53 (s, 1H), 7.52 (s, 1H), 4.66 – 4.59 (m, 2H), 4.17 (dd, *J* = 6.3, 2.2 Hz, 4H), 4.13 (s, 3H), 3.53 (d, *J* = 0.7 Hz, 3H), 2.45 – 2.34 (m, 2H), 1.36 – 1.28 (m, 2H), 1.27 – 1.21 (m, 12H), 0.18 (s, 9H). ^{13}C NMR (75 MHz, $CDCl_3$) δ ppm = 166.52, 166.18, 163.40, 163.31, 150.27, 149.71, 146.00, 145.87, 139.24, 121.60, 121.52, 113.34, 98.75, 98.69, 75.10, 75.07, 64.63, 53.25, 28.40, 19.25, 17.45, 13.18, -1.26. HRMS (ESI$^+$): *m/z* calcd for $C_{29}H_{41}N_2O_6Si$ $[M+H]^+$ 541.2728 found 541.2718.



26

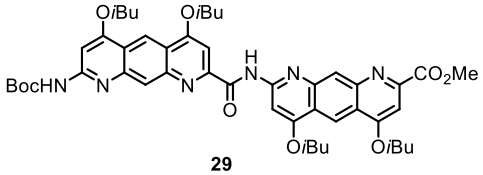
Monomer 26. Diazaanthracene **25** (4.4 g, 8.13 mmol), recrystallized N-bromosuccinimide (1.88 g, 10.5 mmol) and benzoyl peroxide (492 mg, 2 mmol) were dissolved in benzene (40 mL) then, the reaction mixture was let to stir at 65°C. After 12 hours, the reaction mixture was washed with a sodium bisulfite aqueous solution, until a negative starch iodide test for peroxides. Solvent was removed under reduced pressure and the residue was dissolved in dichloromethane, washed with water and brine then, the organic layer was dried over Na_2SO_4, filtered and solvent was removed under reduced pressure. The residue was dissolved in dichloromethane then, methanol was added and dichloromethane was slowly removed by rotary evaporation allowing precipitation of the diazaanthracene. The precipitate was filtered, washed with cold methanol on the filter and dried under vacuum to give **26** (4 g, 79%) as a yellow solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ ppm = 9.27 (s, 1H), 7.50 (d, *J* = 1.8 Hz, 2H), 6.16 (s, 2H), 4.64 – 4.55 (m, 2H), 4.16 – 4.11 (m, 4H), 4.10 (s, 3H), 2.42 – 2.30 (m, *J* = 13.1, 6.7 Hz, 2H), 1.31 – 1.23 (m, *J* = 10.9, 5.5 Hz, 2H), 1.19 (d, *J* = 6.7 Hz, 12H), 0.16 (s, 9H). ^{13}C NMR (75 MHz, $CDCl_3$) δ ppm =

166.47, 166.11, 163.52, 163.43, 151.50, 150.94, 145.22, 145.15, 136.02, 121.89, 121.80, 117.12, 99.41, 99.37, 75.35, 75.32, 64.77, 53.34, 28.39, 25.26, 19.25, 17.43, -1.18. HRMS (ESI$^+$): *m/z* calcd for $C_{29}H_{40}BrN_2O_6Si$ $[M+H]^+$ 619.1833 found 619.1824.



28

Monomer 28. Methyl ester diazaanthracene **27**[8] (1.6 g, 3.2 mmol) was dissolved in a mixture of THF/MeOH/H_2O (30 mL, 8:1:1 vol/vol) and lithium hydroxide monohydrate (270 mg, 6.4 mmol) were added. The reaction mixture was let to stir at room temperature. After 2 hours, the reaction mixture was quenched by addition of an aqueous citric acid solution (5% weight). The organic solvent was removed by rotary evaporation allowing precipitation of the acid diazaanthracene in acidic aqueous solution. The precipitate was collected by filtration and washed with distilled water on the filter. Then, the solid residue was dissolved in dichloromethane, the organic layer was dried over Na_2SO_4, filtered and the solvent was removed under reduced pressure to give **28** as yellow solid (1.52 g, 98 %). ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.15 (s, 1H), 8.41 (s, 1H), 7.74 (s, 1H), 7.54 (s, 1H), 4.17 (d, *J* = 6.4 Hz, 2H), 4.12 (d, *J* = 6.3 Hz, 2H), 2.44 – 2.28 (m, 2H), 1.57 (s, 9H), 1.19 (d, *J* = 6.7 Hz, 12H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.92, 164.17, 163.66, 155.34, 152.55, 150.60, 123.02, 120.93, 119.14, 117.87, 96.75, 92.74, 81.94, 75.95, 75.20, 28.48, 28.39, 19.35, 19.22. HRMS (ESI$^+$): *m/z* calcd for $C_{26}H_{34}N_3O_6$ $[M+H]^+$ 484.2442 found 484.2436.



29

Dimer 29. Amine diazaanthracene **27** (500 mg, 1.26 mmol), acid diazaanthracene **20** (608 mg, 1.26 mmol) and PyBOP (1.31 g, 2.52 mmol) were dissolved in dry chloroform (10 mL). Then, DIEA (0.43 mL, 2.52 mmol) was added and the reaction mixture was let to stir at 45°C. After 12 hours, the reaction mixture was diluted with dichloromethane, washed with a saturated aqueous solution of NH_4Cl, distilled water and brine then, the organic layer was dried over $MgSO_4$, filtered and the solvent was removed under reduced pressure. The residue was dissolved in dichloromethane then, methanol was added and dichloromethane was slowly removed by rotary evaporation allowing precipitation of the dimer. The precipitate was filtered, washed with cold methanol on the filter and dried under vacuum to give **29** (940 mg, 87 %) as a yellow solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ ppm = 11.14 (s, 1H), 9.17 (s, 1H), 9.13 (s, 1H), 8.82 (s, 1H), 8.61 (s, 1H), 8.23 (s, 1H), 7.83 (s, 1H), 7.72 (s, 1H), 7.64 (s, 1H), 7.47 (s, 1H), 4.22 – 4.09 (m, 11H), 2.45 – 2.32 (m, 4H), 1.59 (s, 9H), 1.25 – 1.16 (m, 24H). ^{13}C NMR (75 MHz, $CDCl_3$) δ ppm = 166.48, 163.98, 163.82, 163.39, 154.90, 153.62, 152.89, 151.77, 150.86, 147.98, 147.32, 147.15, 146.98, 126.73, 125.27, 120.81, 120.42, 119.57, 119.28, 116.67, 116.52, 98.22, 95.48, 93.54, 92.58, 81.60, 75.18, 75.07, 74.95, 53.42, 28.45, 19.35, 19.27. HRMS (ESI$^+$): *m/z* calcd for $C_{48}H_{59}N_6O_9$ $[M+H]^+$ 863.4338 found 863.4344.

3. Solution studies by NMR

3.1 NMR study of monomer 9

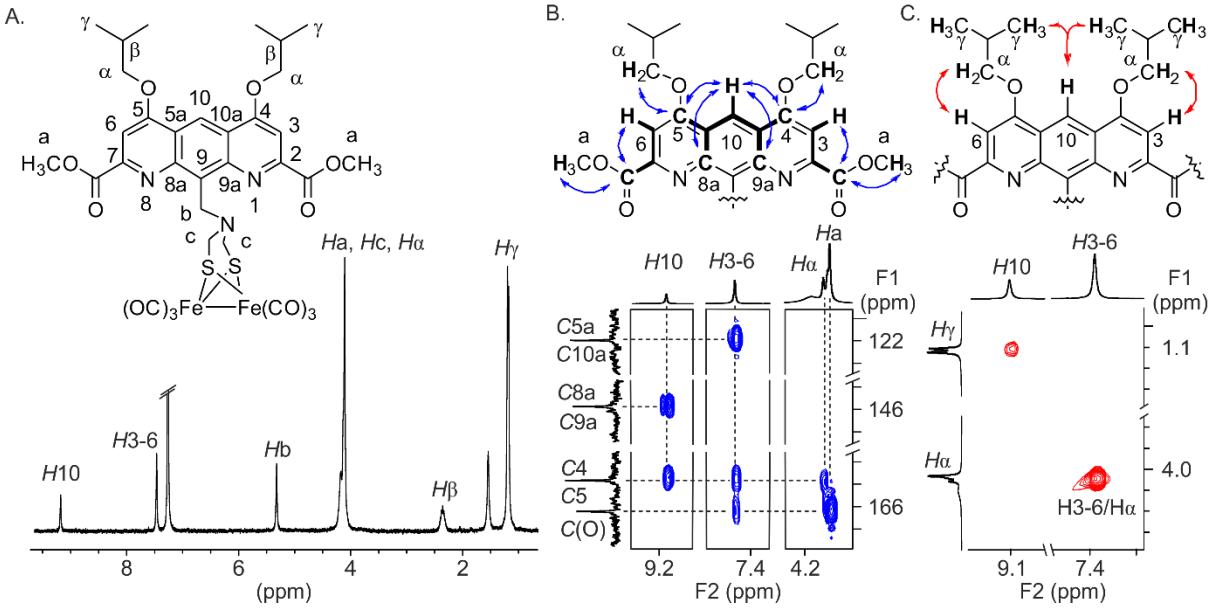


Figure S1. (A) Full ^{1}H NMR spectrum (400 MHz) at 298 K of monomer **9** in $CDCl_3$ with signals attribution. (B) Excerpt of HMBC spectrum (400 MHz) at 298 K of monomer **9** in $CDCl_3$. (C) Excerpt of ^{1}H-^{1}H NOESY spectrum (400 MHz, τ = 300 ms) at 298 K of monomer **9** in $CDCl_3$ showing correlations between aromatic and lateral chain protons.

3.2 NMR study of monomer 16

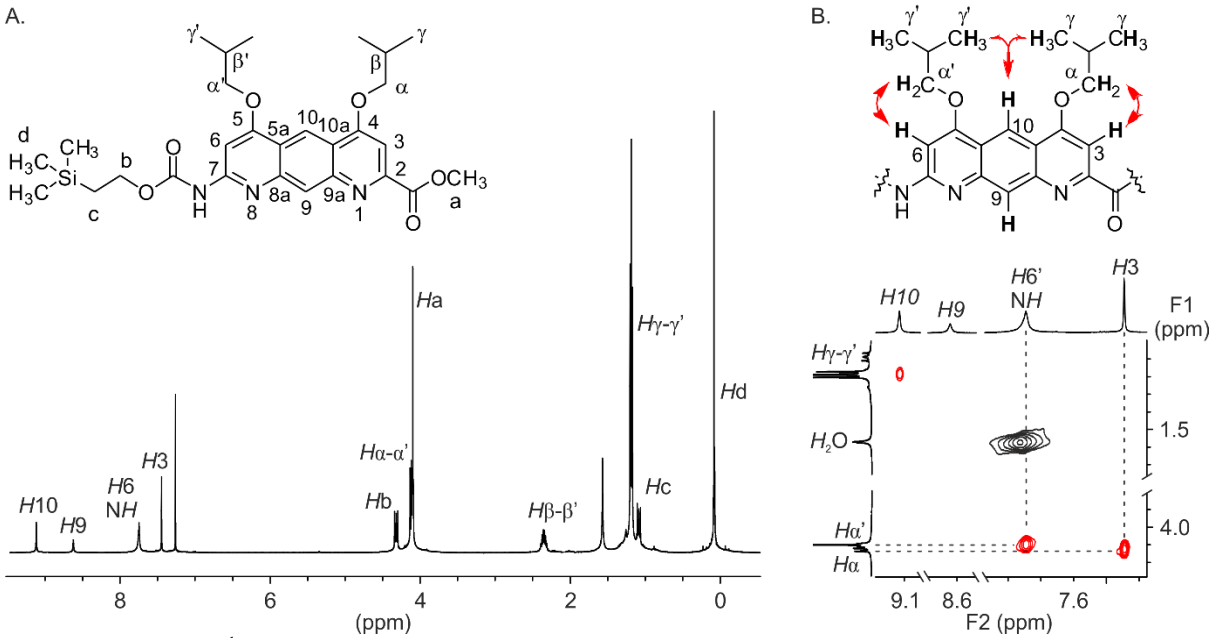


Figure S2. (A) Full ^{1}H NMR spectrum (400 MHz) at 298 K of monomer **16** in $CDCl_3$ with signals attribution. (B) Excerpt of ^{1}H-^{1}H NOESY spectrum (400 MHz, τ = 300 ms) at 298 K of monomer **16** in $CDCl_3$ showing correlations between aromatic and lateral chain protons.

3.3 NMR study of dimer 20

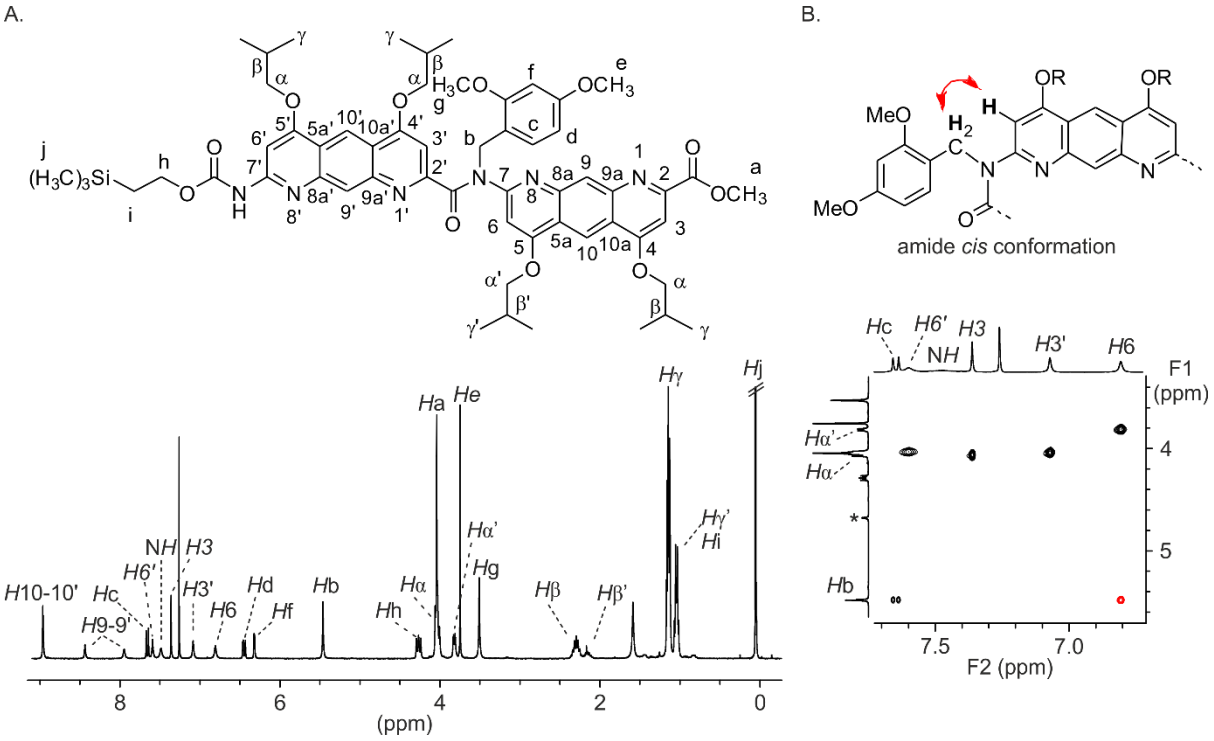


Figure S3. (A) Full ^{1}H NMR spectrum (400 MHz) at 298 K of dimer **20** in $CDCl_3$ with signals attribution. (B) Excerpt of ^{1}H-^{1}H NOESY spectrum (400 MHz, τ = 300 ms) at 298 K of dimer **20** in $CDCl_3$ showing the correlation between the aromatic proton *H*6 and the benzylic protons *H*b in red due to tertiary amide *cis* conformation.

3.4 NMR comparison of dimer 20, tetramer 22 and oligomer 4

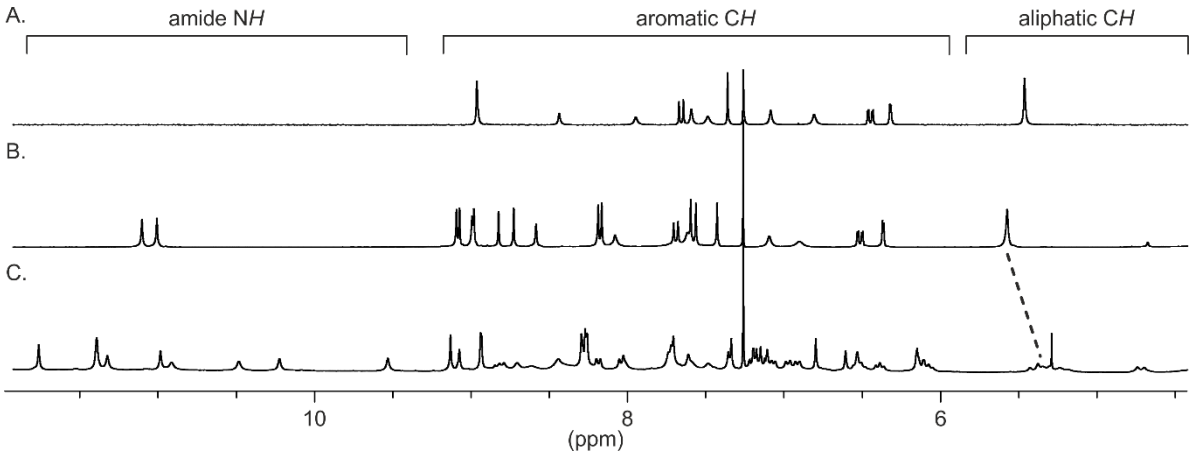


Figure S4. Part of ^{1}H NMR spectrum (300 MHz) at 298 K in $CDCl_3$ of dimer **20** (A), tetramer **22** (B) and oligomer **4** (C) with appearance of benzyl protons anisochronicity (dotted line).

3.5 NMR study of oligomer 5

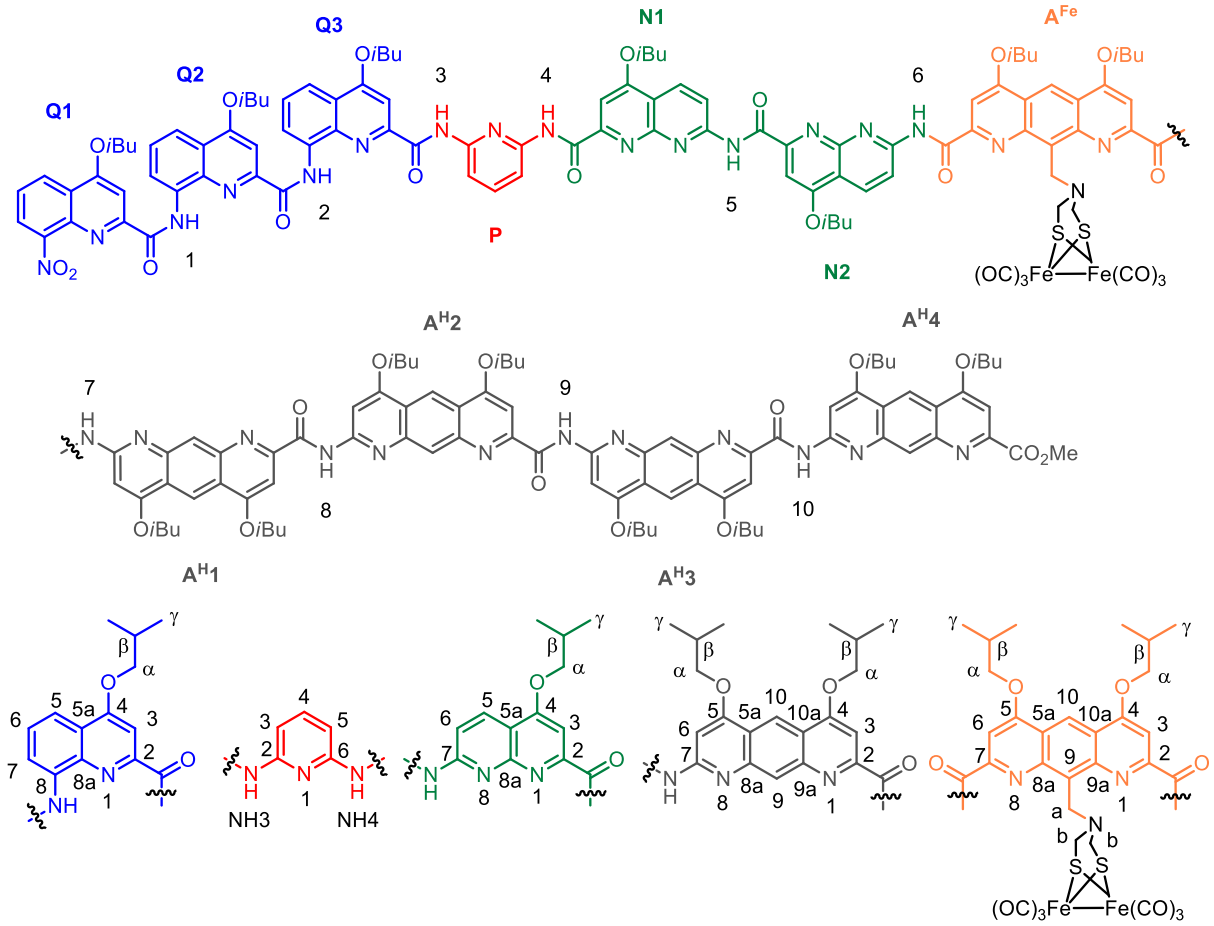


Figure S5. Monomers and atoms numbering for oligomer **5**.

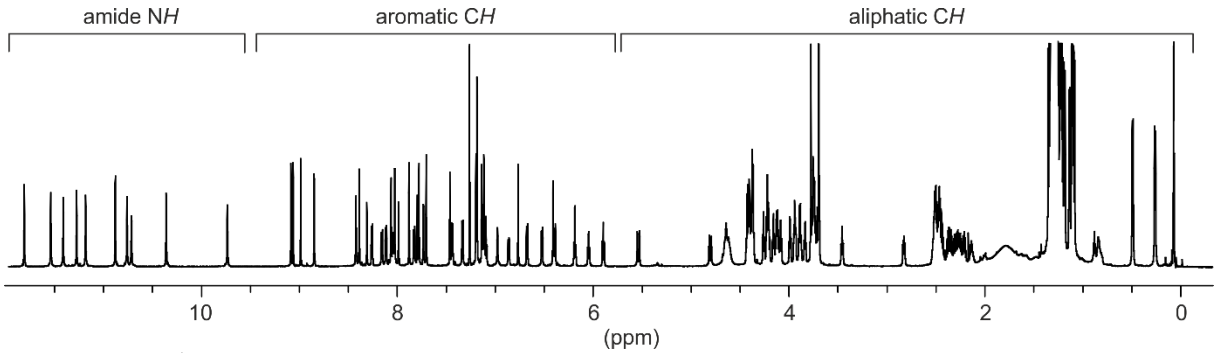


Figure S6. Full ^{1}H NMR spectrum (700 MHz) at 298 K of oligomer **5** in $CDCl_3$.

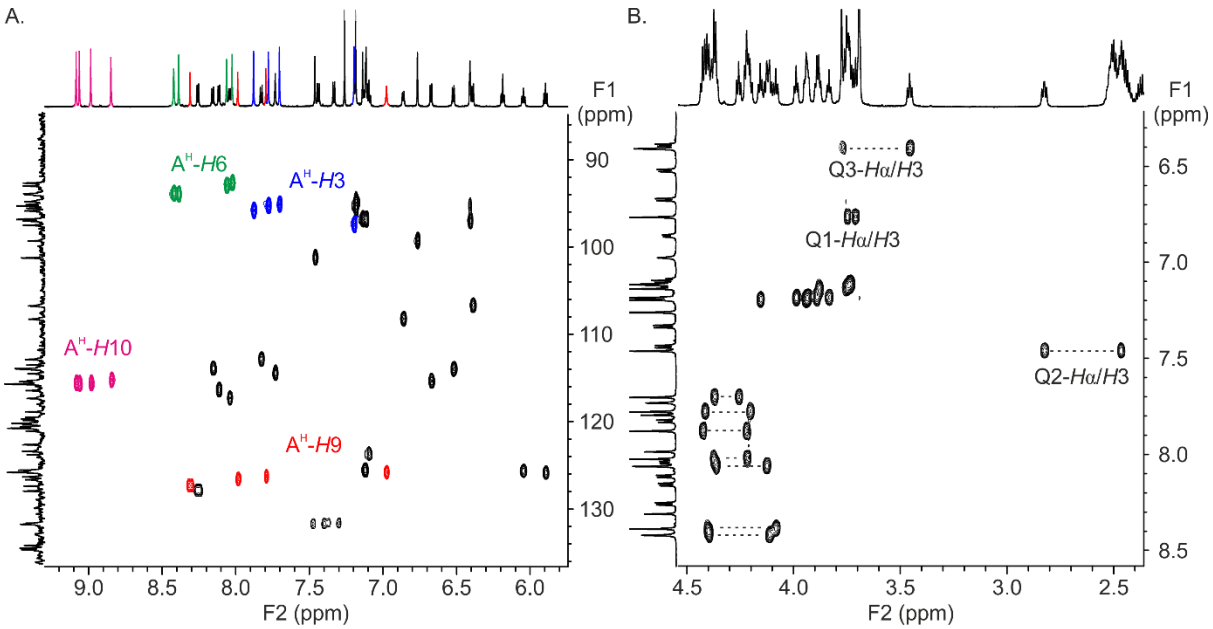


Figure S7. (A) Excerpt of HMBC spectrum (700 MHz) at 298 K of oligomer **5** in $CDCl_3$ showing the different aromatic protons from the A^H units. (B) Excerpt of ^1H-^1H NOESY spectrum (700 MHz, τ = 300 ms) at 298 K of oligomer **5** in $CDCl_3$ showing correlations between lateral chain protons *H*α due to anisochronicity.

Table S1. Partial attribution of ^{1}H and ^{13}C chemical shifts for oligomer **5** in CDCl3, measured at 700 MHz and 176 MHz, respectively, 298 K.

	Chemical shift (ppm)			Chemical shift (ppm)			Chemical shift (ppm)	
	^{1}H	^{13}C		^{1}H	^{13}C		^{1}H	^{13}C
Q1-CH7	7.11 (d)	125.7	*NH3*	9.73 (s)			11.27 (s)	
Q1-CH6	7.09 (t)	123.5	*P-CH3*	6.38 (d)	106.7	*NH8,9,10*	10.80 (s)	
Q1-CH5	8.25 (d)	127.7	*P-CH4*	6.18 (t)	137.1		10.35 (s)	
Q1-CH3	6.76 (s)	99.2	*P-CH5*	6.85 (d)	108.2	*A^{H}1-CH6*	8.02 (s)	92.6
Q1-C4		162.3	*NH4*	10.71 (s)			8.06 (s)	92.7
Q1-C10		123.3	*N1-CH3*	7.13 (s)	96.7	*A^{H}2,3,4-CH6*	8.42 (s)	93.7
Q1-CHα	3.70 (t) 3.74 (t)	74.9	*N1-CH5*	7.33 (d)	131		8.38 (s)	93.8
NH1	11.80 (s)		*N1-CH6*	7.82 (d)	112.8		7.70 (s)	95
Q2-CH7	8.11 (d)	116.6	*N1-C5a*		113.5	*A^{H}1,2,3-CH3*	7.77 (s)	95.1
Q2-CH6	5.89 (t)	125.9	*N1-CH_2α*	3.75 (t)	75		7.87 (s)	95.7
Q2-CH5	6.68 (d)	115.2	*NH5*	11.40 (s)		*A^{H}4-CH3*	7.19 (s)	97.4
Q2-CH3	7.46 (s)	101.3	*N2-CH3*	7.11 (s)	96.8		8.31 (s)	127.3
Q2-C4		163.4	*N2-CH5*	7.44 (d)	131		7.98 (s)	126.5
Q2-C10		122.2	*N2-CH6*	8.15 (d)	113.8	*A^{H}1,2,3,4-CH9*	7.79 (s)	126.2
Q2-CHα	2.82 (t) 2.46 (t)	75	*N2-C5a*		113.9		6.97 (s)	125.7
NH2	11.53		*N2-CH_2α*	3.74 (t)	75		9.08 (s)	115.5
Q3-CH7	8.04 (d)	117.3	*NH6*	11.18 (s)			9.06 (s)	115.6
Q3-CH6	6.04 (t)	125.5	*A^{Fe}-CH3/CH6*	7.18 (s)	95	*A^{H}1,2,3,4-CH10*	8.98 (s)	115.5
Q3-CH5	6.52 (d)	113.9	*A^{Fe}-CH10*	7.73 (s)	114.5		8.84(s)	115.2
Q3-CH3	6.40 (s)	95.2		4.80 (d)		CH_3-Ester	3.69 (s)	52.9
Q3-C4		161.5	*A^{Fe}-CH_2a*	5.53 (d)	50.5			
Q3-C10		120.5	*A^{Fe}-CH_2b*	4.63 (m)	54.5			
Q3-CHα	3.45 (t) 3.76 (t)	74.6	*NH7*	10.75 (s)				

3.6 Full Width at Half Maximum of carbonyl ligand signals

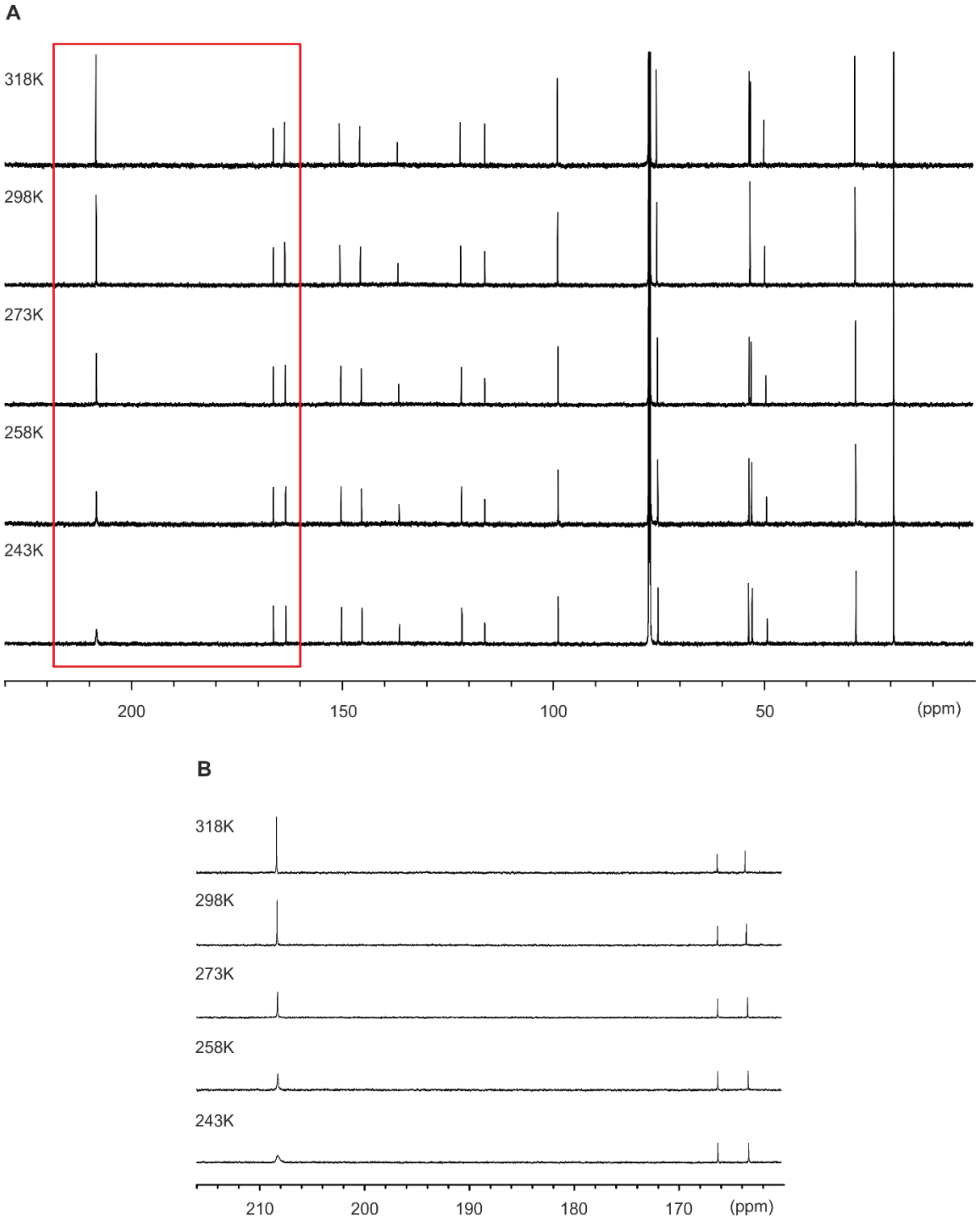


Figure S8. (A) Full ^{13}C NMR spectra (176 MHz) of monomer **9** in $CDCl_3$ at variable temperatures. (B) Excerpt of ^{13}C NMR spectra (176 MHz) of monomer **9** in $CDCl_3$ at variable temperatures.

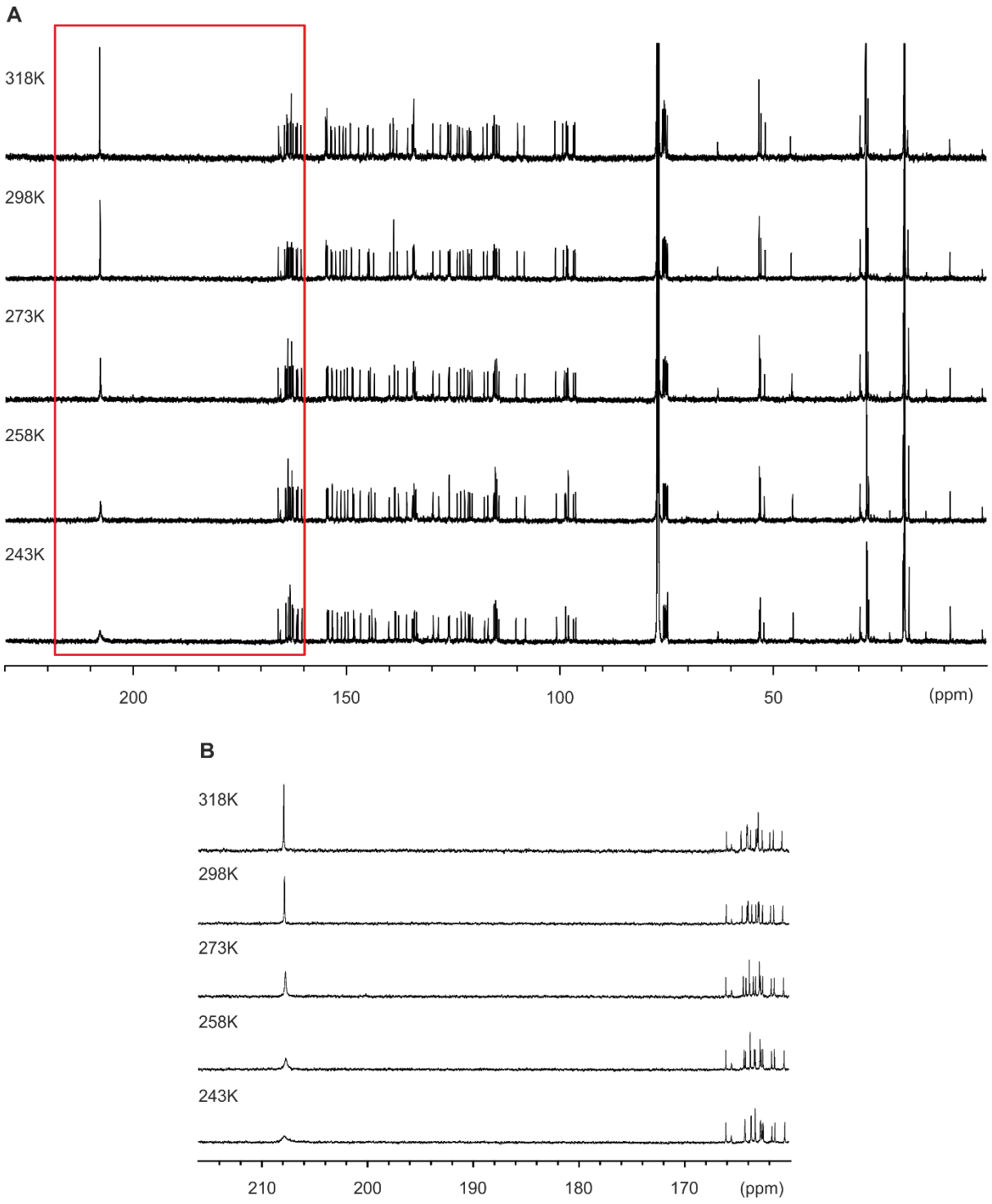


Figure S9. (A) Full ^{13}C NMR spectra (176 MHz) of oligomer **1** in $CDCl_3$ at variable temperatures. (B) Excerpt of ^{13}C NMR spectra (176 MHz) of oligomer **1** in $CDCl_3$ at variable temperatures.

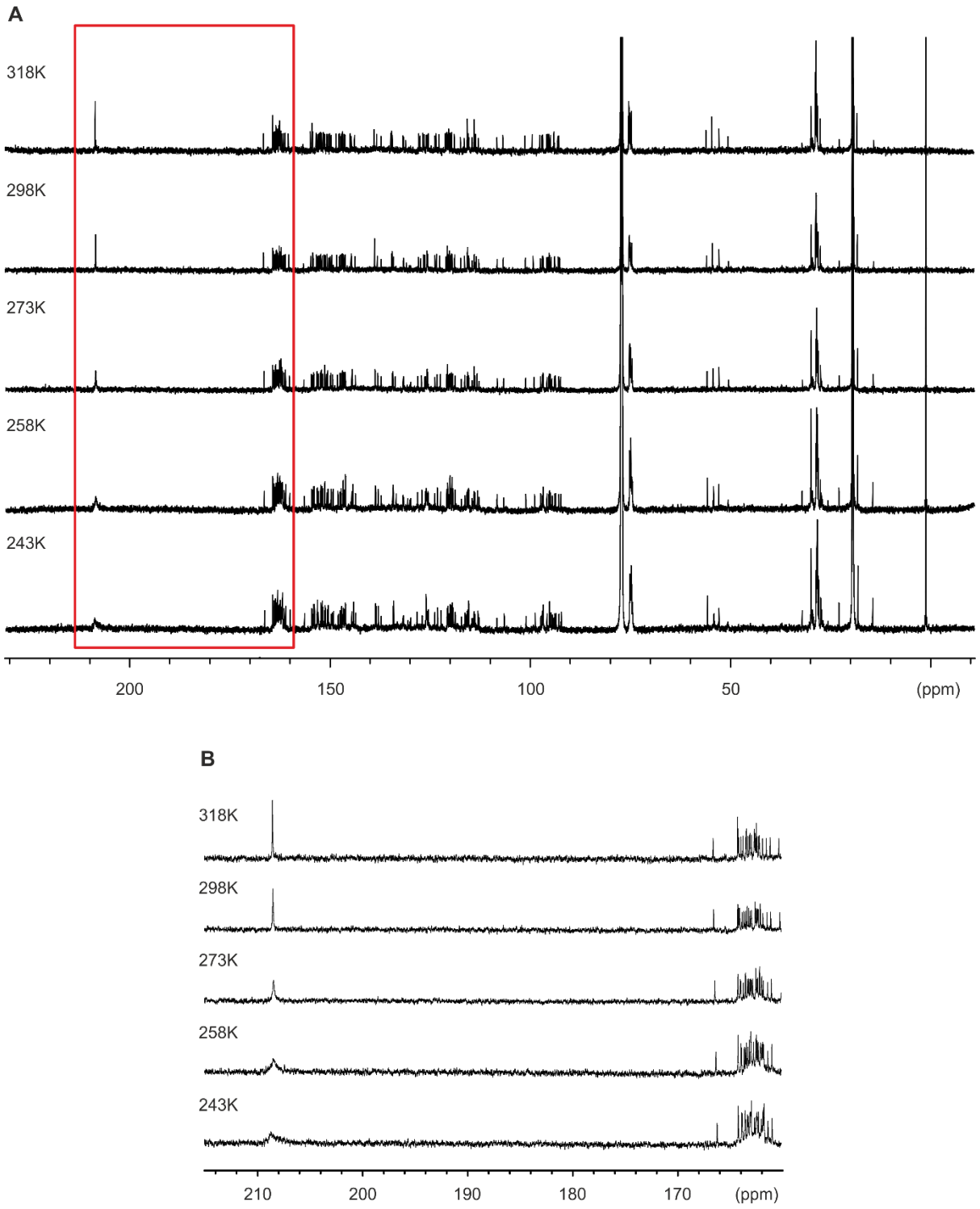


Figure S10. (A) Full ^{13}C NMR spectra (176 MHz) of oligomer **5** in $CDCl_3$ at variable temperatures. (B) Excerpt of ^{13}C NMR spectra (176 MHz) of oligomer **5** in $CDCl_3$ at variable temperatures.

4. Solid state X-Ray Crystallography

4.1 X-Ray crystallographic data for compound 1

Table S2. Crystal data and refinement details for compound **1**.

Identification code	**1**
Chemical formula	$C_{107}H_{105}Cl_9Fe_2N_{19}O_{23}S_2$
Formula weight	2159.96
Temperature (K)	130
Wavelength (Å)	1.54178
Crystal system	monoclinic
Space group	C2/c
Unit cell dimensions (a,b,c,α,β,γ) (Å, °)	42.379, 22.277, 31.801, 90.0, 98.36, 90.0
Volume ($Å^3$)	29703.8
Z	8
Density (calculated)	1.127
Absorption coefficient	3.826
Absorption correction	multiscan
Crystal size (mm)	0.10, 0.10, 0.10
Index ranges	$-39 \leqslant h \leqslant 40$, $-21 \leqslant k \leqslant 16$, $-22 \leqslant l \leqslant 30$
Completeness to theta = 22.72°	0.988
Reflections collected	46092
Reflections observed [I > 2σ(I)]	13285
R_{int}	0.1018
Data/parameters/restrains	13285/1474/27
Goodness-of-fit on F^2	1.132
Final R indices [I > 2σ(I)]	0.1284
R indices (all data)	0.1747
Largest diff. peak and hole	0.47/-0.46
CCDC #	2031551

*SQUEEZE procedure was used to remove severely disordered solvent molecules

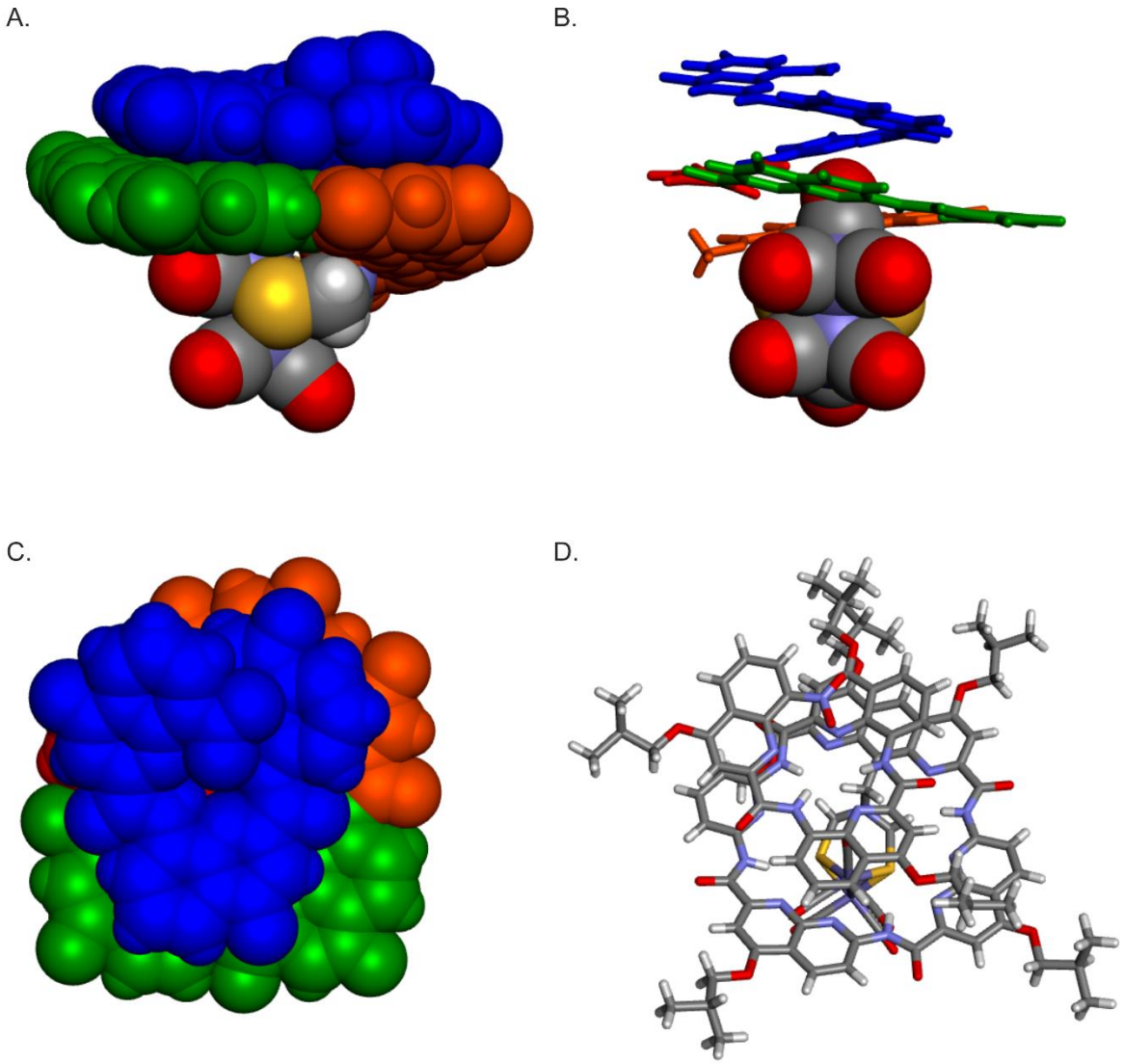


Figure S11. Crystal structure views of oligomer **1**. (A) side view, (B) front view, (C) view from above in CPK representations. Monomers are color coded as in manuscript and isobutoxy side chains are omitted for clarity. (D) view from above in tube representation where isobutoxy side chains are shown and atoms are color coded in grey for carbon, red for oxygen, blue for nitrogen, white for hydrogen, yellow for sulfur and purple for iron.

4.2 X-Ray crystallographic data for compound 3

Table S3. Crystal data and refinement details for compound **3**.

Identification code	**3**
Chemical formula	C148 H150 Cl3 Fe2 N24 029 S2
Formula weight	2890
Temperature (K)	100
Wavelength (Å)	0.8100
Crystal system	triclinic
Space group	P-1
Unit cell dimensions (a,b,c,α,β,γ) (Å, °)	17.679, 22.049, 25.574, 72.80, 73.10, 79.75
Volume ($Å^3$)	9065.6
Z	2
Density (calculated)	1.102
Absorption coefficient	0.413
Absorption correction	None
Crystal size (mm)	0.10, 0.05, 0.07
Index ranges	-19 < h < 19, -24 < k < 24, -28 < l < 28
Completeness to theta = 27.06°	0.913
Reflections collected	94230
Reflections observed [I > 2σ(I)]	15839
R_{int}	0.0576
Data/parameters/restrains	24578/1917/1707
Goodness-of-fit on F^2	1.367
Final R indices [I > 2σ(I)]	0.1129
R indices (all data)	0.1384
Largest diff. peak and hole	1.14/-0.45
CCDC #	2031556

*SQUEEZE procedure was used to remove severely disordered solvent molecules

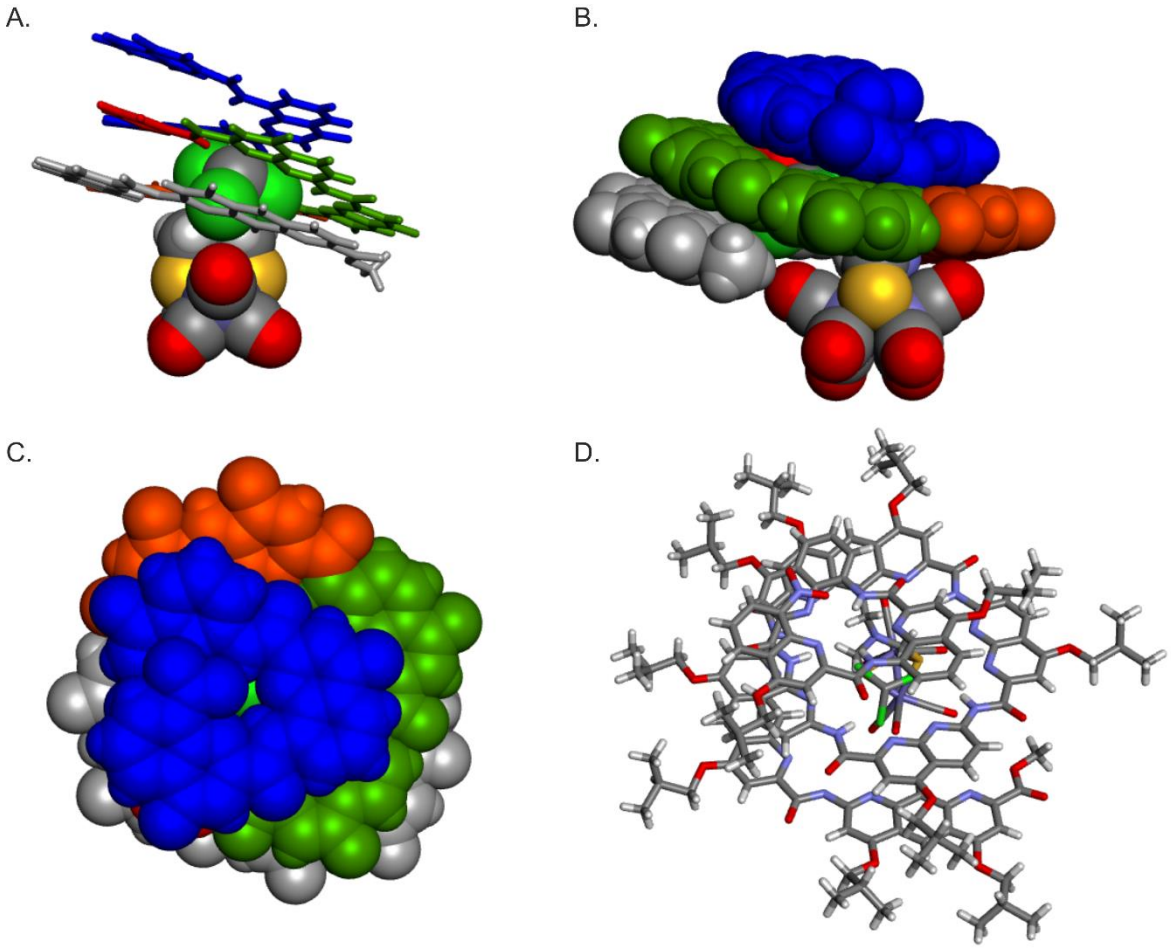


Figure S12. Crystal structure views of oligomer **3**. (A) front view where the aromatic backbone is shown in color coded tube representation whereas the metal complex is show in CPK representation. (B) side view in CPK representation. (C) view from above in CPK representation. Monomers are color coded as in manuscript and isobutoxy side chains are omitted for clarity. (D) view from above in tube representation where isobutoxy side chains are shown and atoms are color coded in grey for carbon, red for oxygen, blue for nitrogen, white for hydrogen, yellow for sulfur and purple for iron.

4.3 X-Ray crystallographic data for compound 4

Table S4. Crystal data and refinement details for compound **4**.

Identification code	**4**
Chemical formula	C198 H204 Fe2 N30 O37 S2
Formula weight	4010.48
Temperature (K)	100
Wavelength (Å)	1.54178
Crystal system	triclinic
Space group	P-1
Unit cell dimensions (a,b,c,α,β,γ) (Å, °)	26.612, 29.084, 36.118, 83.26, 82.98, 68.18
Volume ($Å^3$)	25678
Z	4
Density (calculated)	1.037
Absorption coefficient	2.15
Absorption correction	multiscan
Crystal size	0.10, 0.10, 0.01
Index ranges	-20 < h < 24, -22 < k < 26, -29 < l < 32
Completeness to theta = 44.28°	0.897
Reflections collected	35867
Reflections observed [I > 2σ(I)]	9759
R_{int}	0.1147
Data/parameters/restrains	35867/4990/8374
Goodness-of-fit on F^2	1.088
Final R indices [I > 2σ(I)]	0.1170
R indices (all data)	0.2194
Largest diff. peak and hole	+0.27/-0.26
CCDC #	2031552

*SQUEEZE procedure was used to remove severely disordered solvent molecules

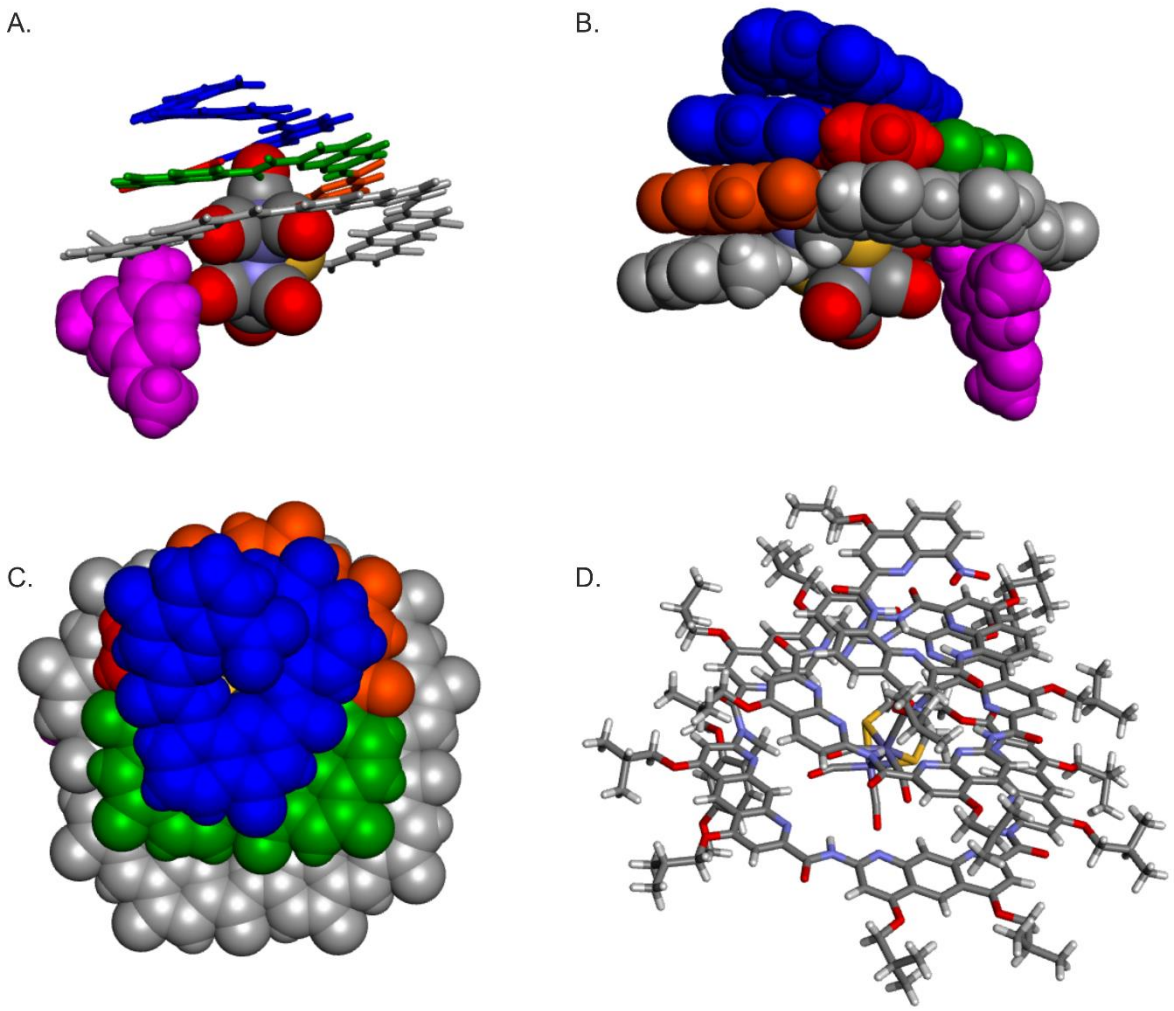


Figure S13. Crystal structure views of oligomer **4**. (A) front view where the aromatic backbone is shown in color coded tube representation whereas the metal complex and DMB group are shown in CPK representation. (B) side view in CPK representation. (C) view from above in CPK representation. Monomers are color coded as in manuscript and isobutoxy side chains are omitted for clarity. (D) view from above in tube representation where isobutoxy side chains are shown and atoms are color coded in grey for carbon, red for oxygen, blue for nitrogen, white for hydrogen, yellow for sulfur and purple for iron.

4.4 X-Ray crystallographic data for compound 5

Table S5. Crystal data and refinement details for compound **5**.

Identification code	**5**
Chemical formula	C195 H198 Cl13 Fe2 N30 O35 S2
Formula weight	3733.12
Temperature (K)	130
Wavelength (Å)	1.54178
Crystal system	triclinic
Space group	P-1
Unit cell dimensions (a,b,c,α,β,γ) (Å, °)	17.496, 21.656, 33.846, 97.71, 104.52, 97.62
Volume ($Å^3$)	12116
Z	2
Density (calculated)	1.023
Absorption coefficient	1.744
Absorption correction	multiscan
Crystal size	0.20, 0.20, 0.2
Index ranges	-15< h <15, -19< k <19, -30< l < 30
Completeness to theta = 51.33°	0.987
Reflections collected	78733
Reflections observed [I > 2σ(I)]	18810
R_{int}	0.1429
Data/parameters/restrains	18810/2417/231
Goodness-of-fit on F^2	0.85
Final R indices [I > 2σ(I)]	0.0890
R indices (all data)	0.1555
Largest diff. peak and hole	+0.44/-0.32
CCDC #	2031555

*SQUEEZE procedure was used to remove severely disordered solvent molecules

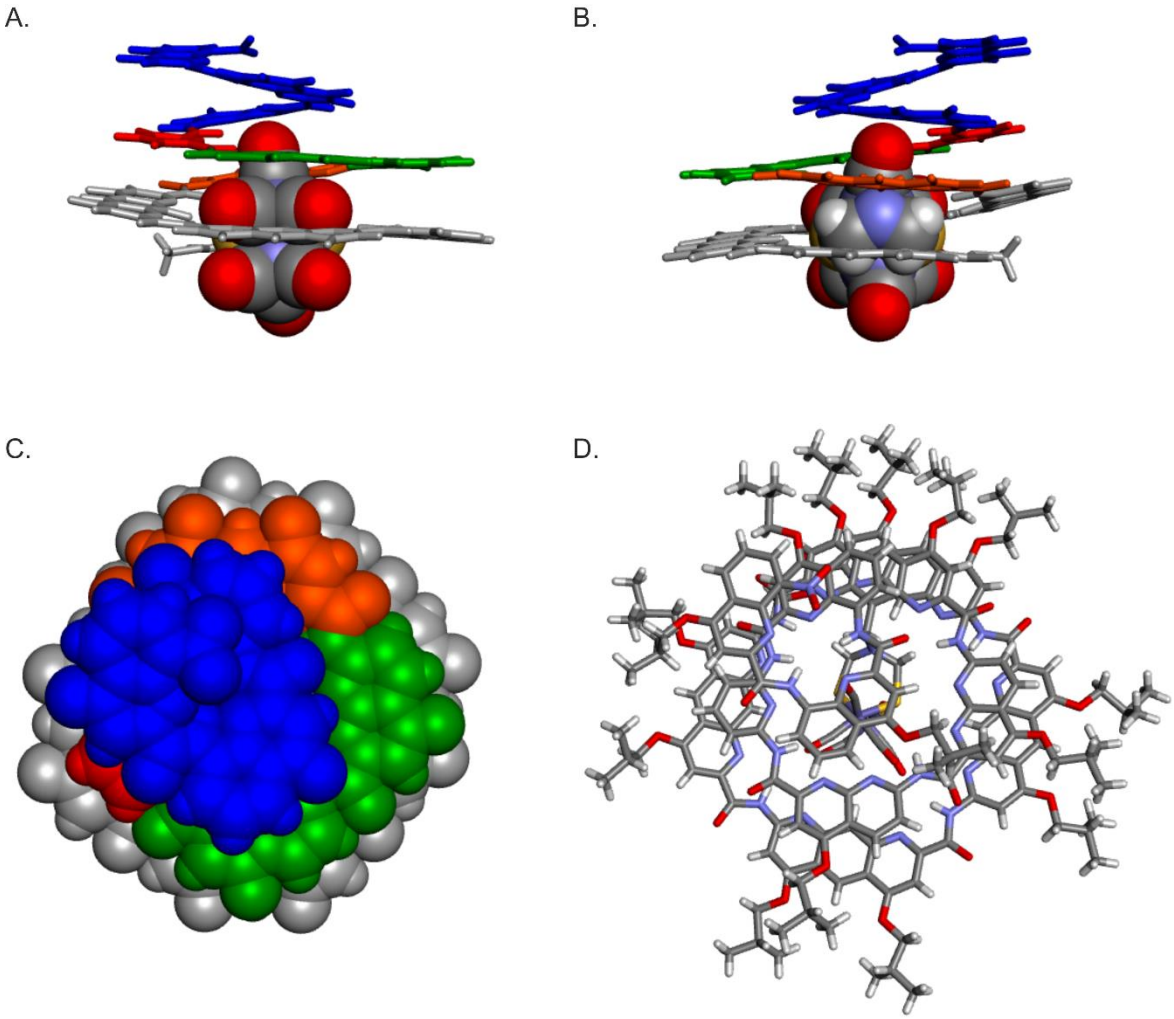


Figure S14. Crystal structure views of oligomer **5**. (A) front view and (B) back view where the aromatic backbone is shown in color coded tube representation whereas the metal complex is shown in CPK representation. (C) view from above in CPK representation. Monomers are color coded as in manuscript and isobutoxy side chains are omitted for clarity. (D) view from above in tube representation where isobutoxy side chains are shown and atoms are color coded in grey for carbon, red for oxygen, blue for nitrogen, white for hydrogen, yellow for sulfur and purple for iron.

4.5 X-Ray crystallographic data for compound 9

Table S6. Crystal data and refinement details for compound **9**.

Identification code	**9**
Chemical formula	C33 H33 Fe2 N3 O12 S2
Formula weight	839.44
Temperature (K)	100
Wavelength (Å)	0.8000
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions (a,b,c,α,β,γ) (Å, °)	11.614, 11.913, 14.995, 90.34, 100.67, 114.20
Volume ($Å^3$)	1851.9
Z	2
Density (calculated)	1.505
Absorption coefficient	1.329
Absorption correction	none
Crystal size (mm)	0.10, 0.050, 0.02
Index ranges	-12 < h < 12, -12 < k < 12, -15 < l < 15
Completeness to theta = 24.895°	0.882
Reflections collected	3993
Reflections observed [I > 2σ(I)]	3617
R_{int}	0.0595
Data/parameters/restrains	3993/507/465
Goodness-of-fit on F^2	1.039
Final R indices [I > 2σ(I)]	0.0576
R indices (all data)	0.0618
Largest diff. peak and hole	0.83/-0.72
CCDC #	2031550

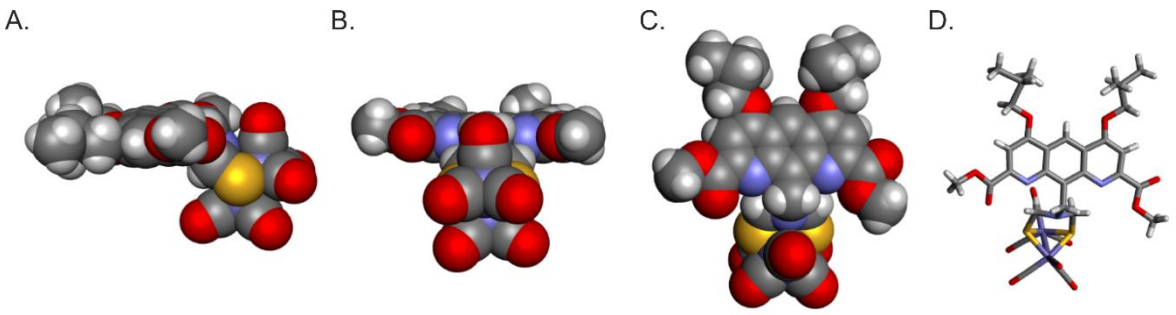


Figure S15. Crystal structure views of A^{Fe} monomer **9**: (A) side view in CPK representations, (B) front view in CPK representations, view from above (C) in CPK representations and (D) in tube representation.

5. References

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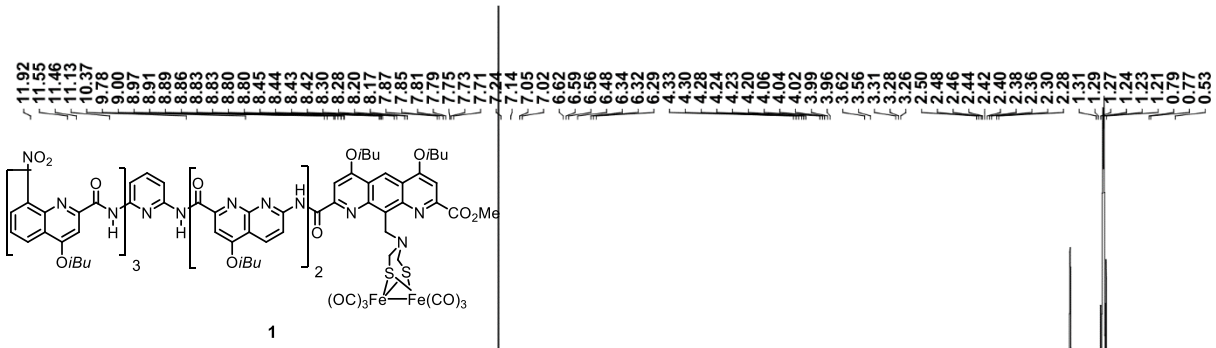
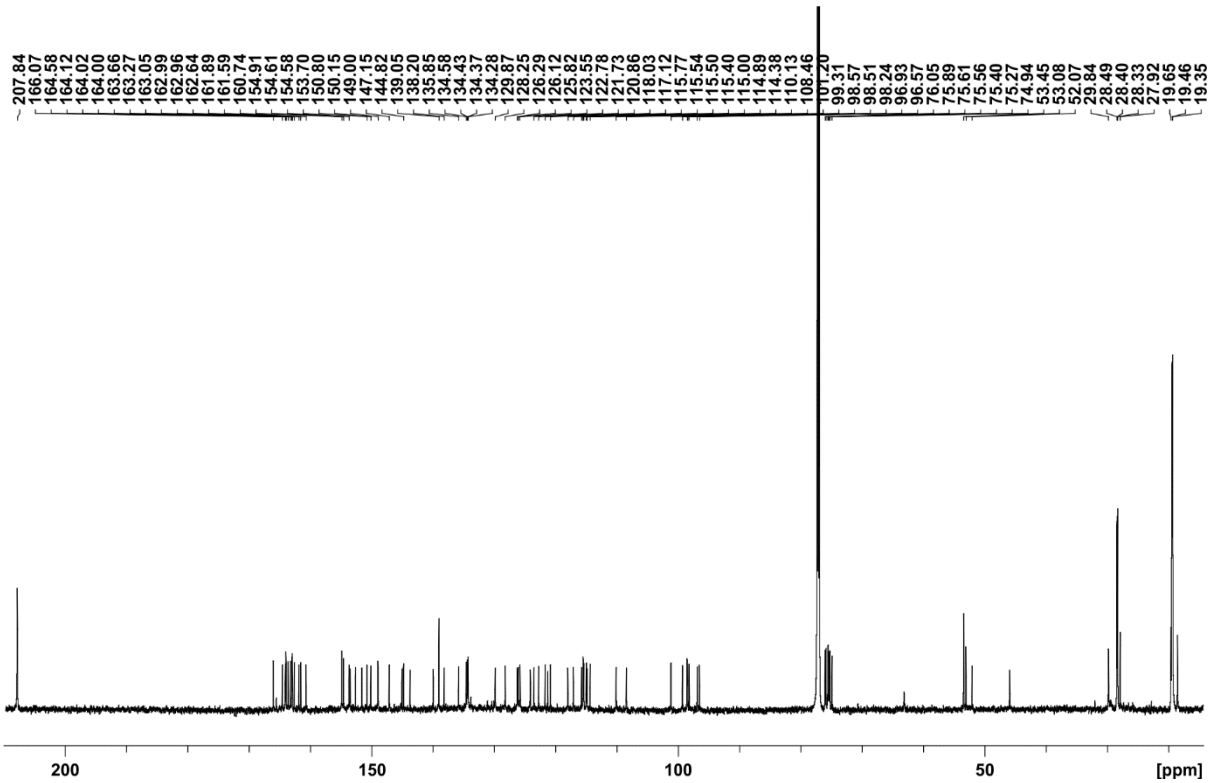
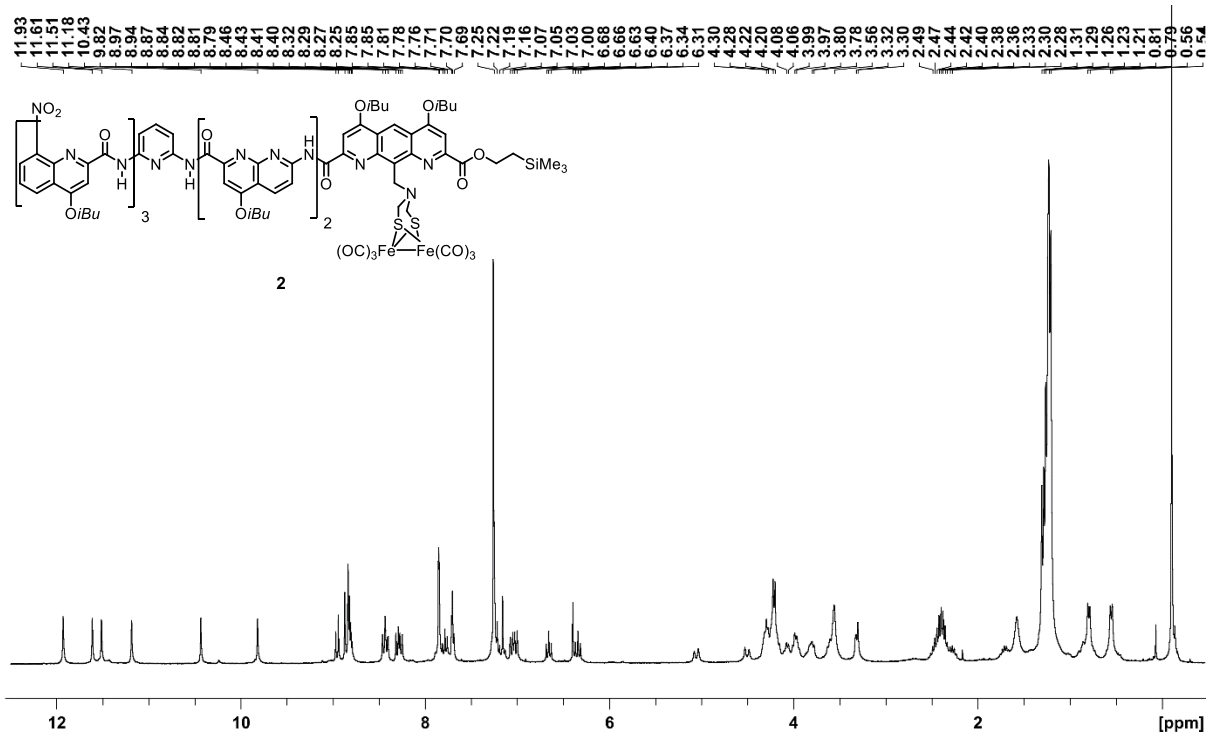
6. ^{1}H NMR and ^{13}C NMR spectra of new synthetic compounds



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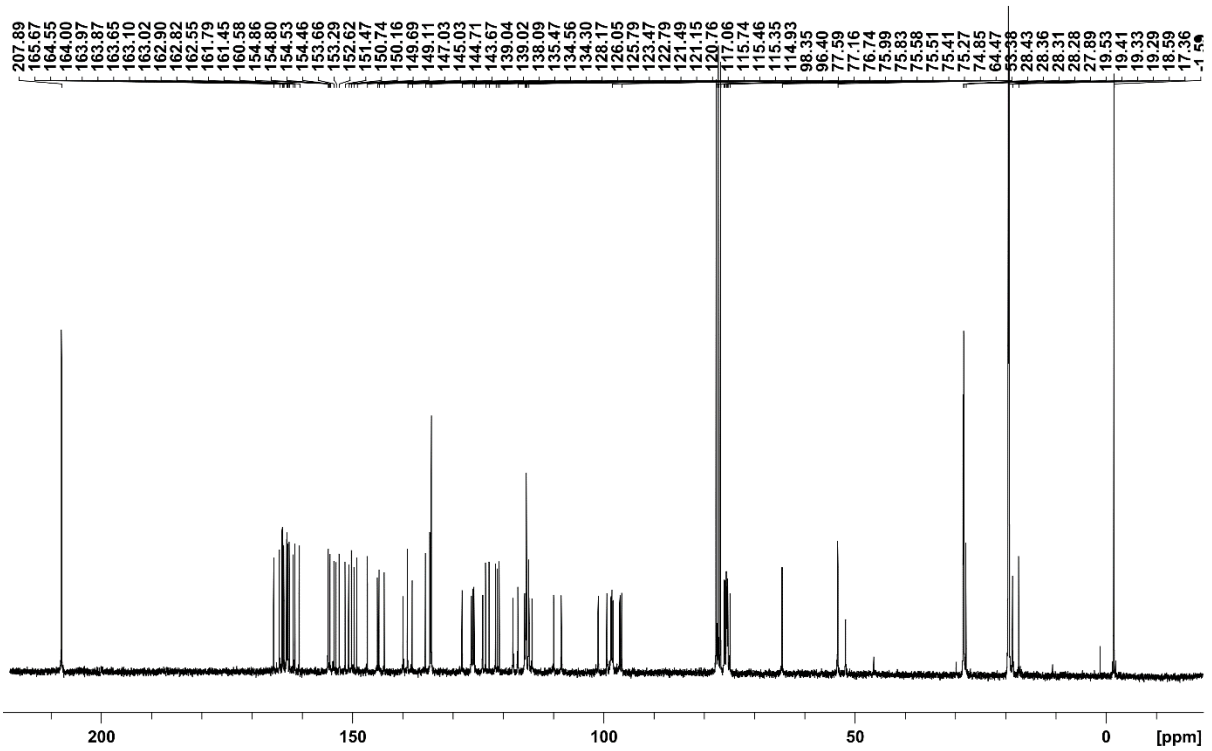
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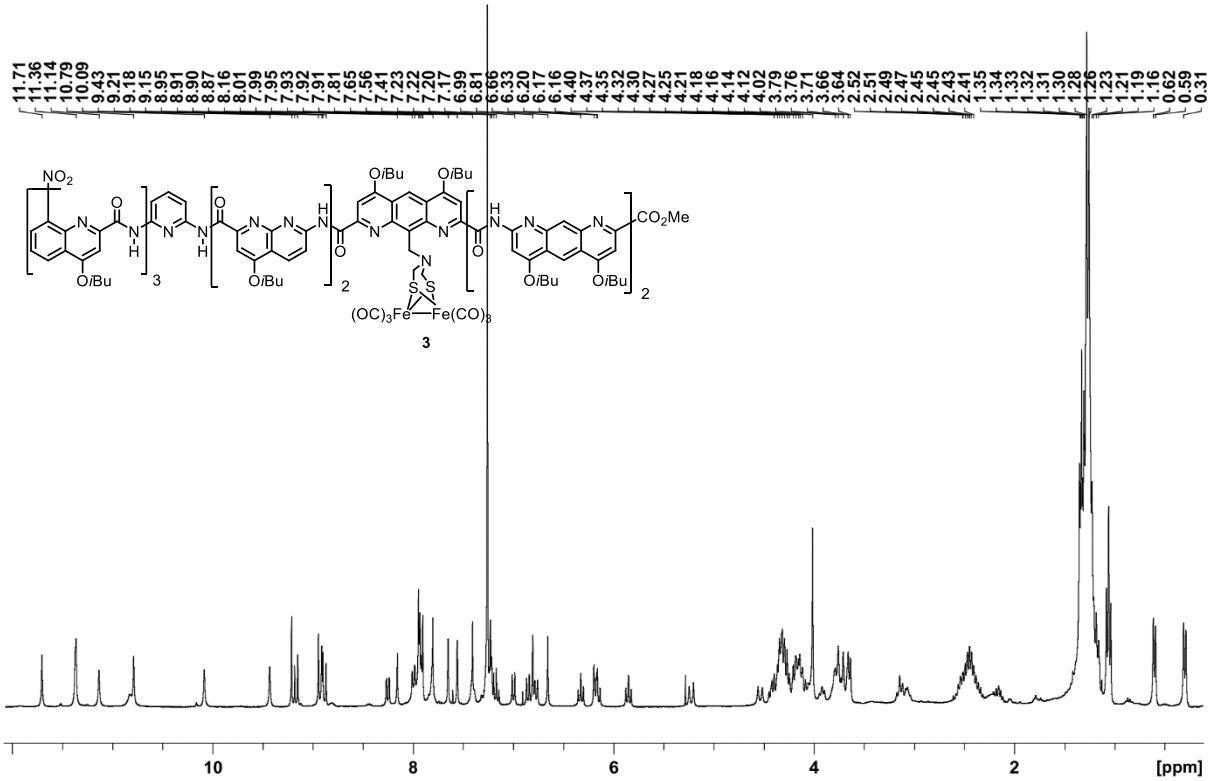
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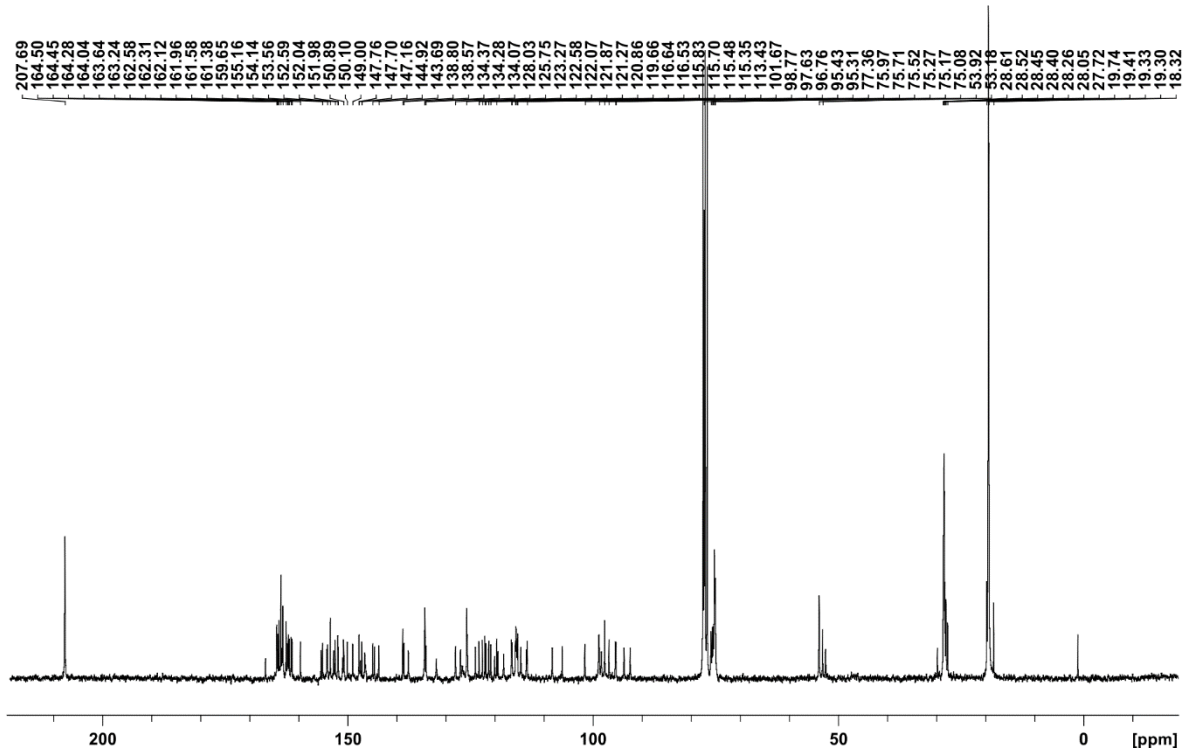
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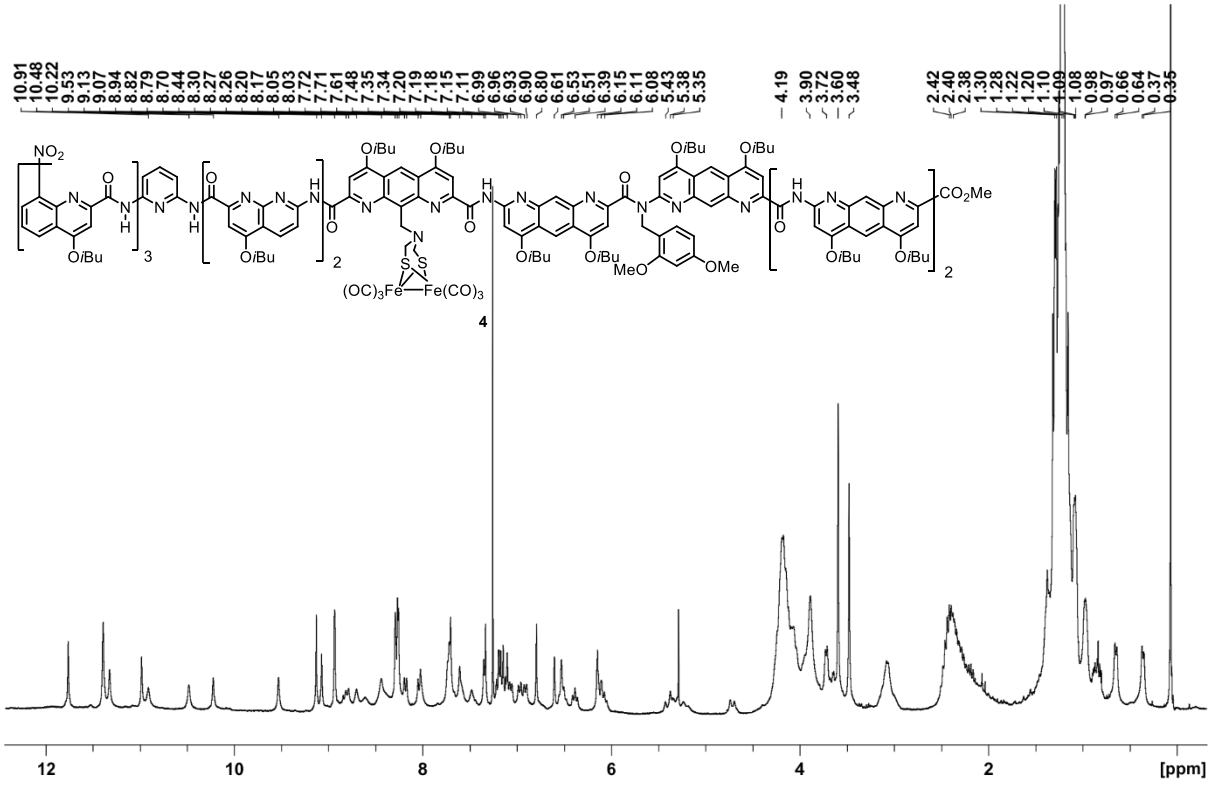
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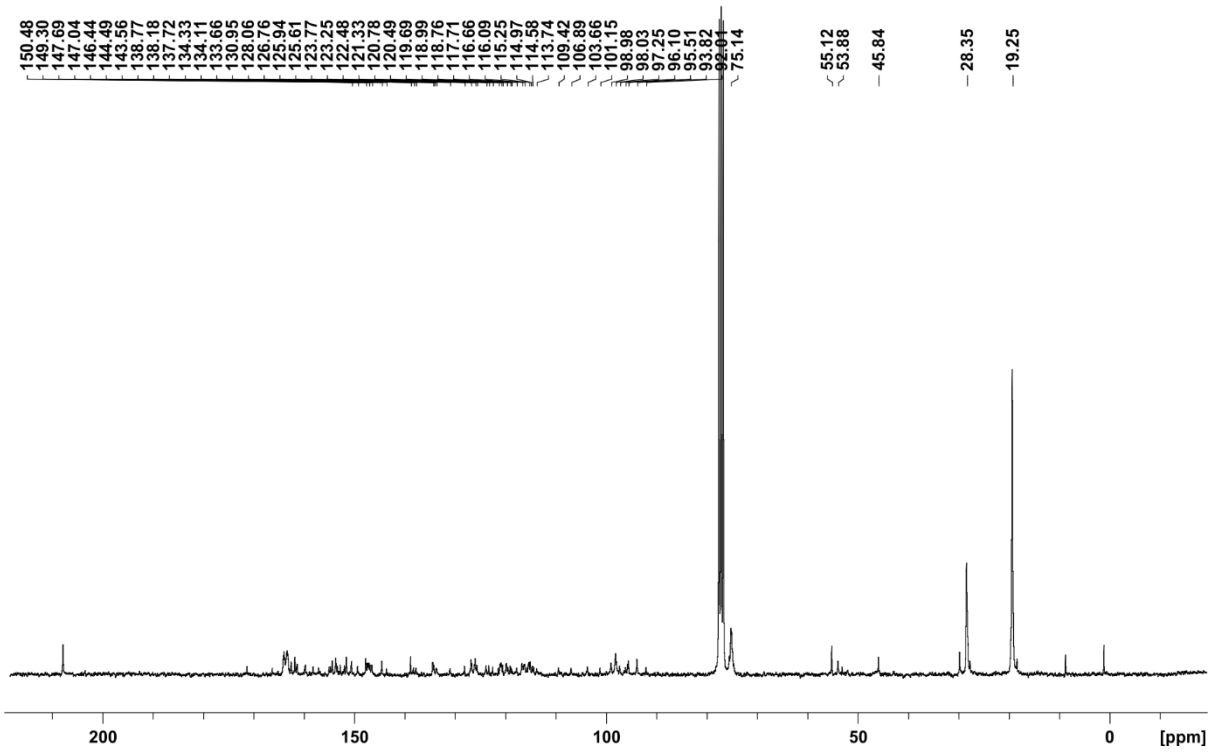
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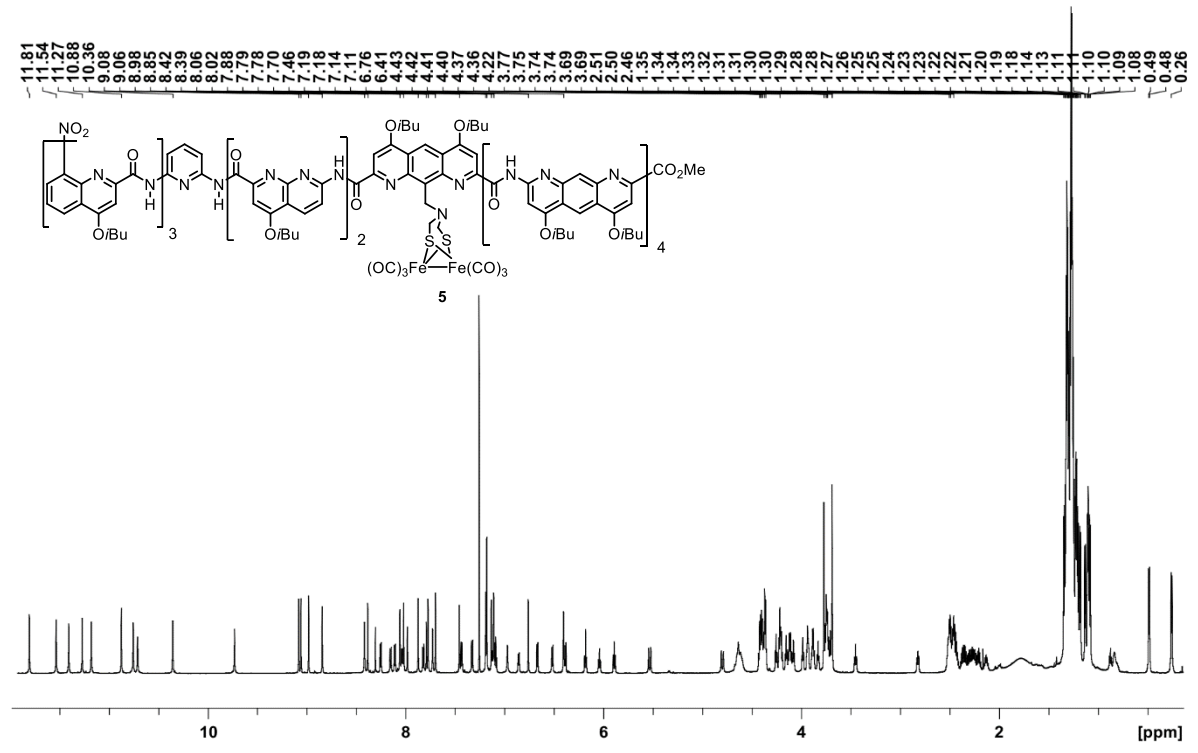
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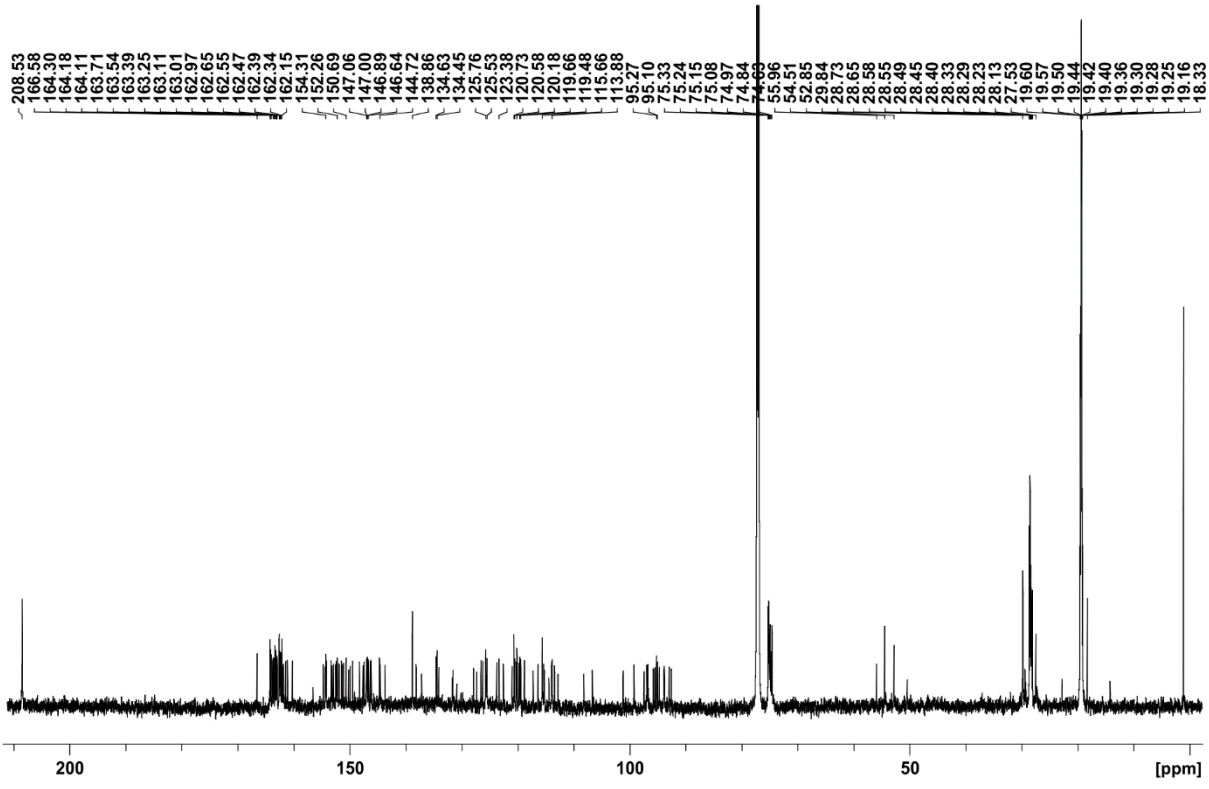
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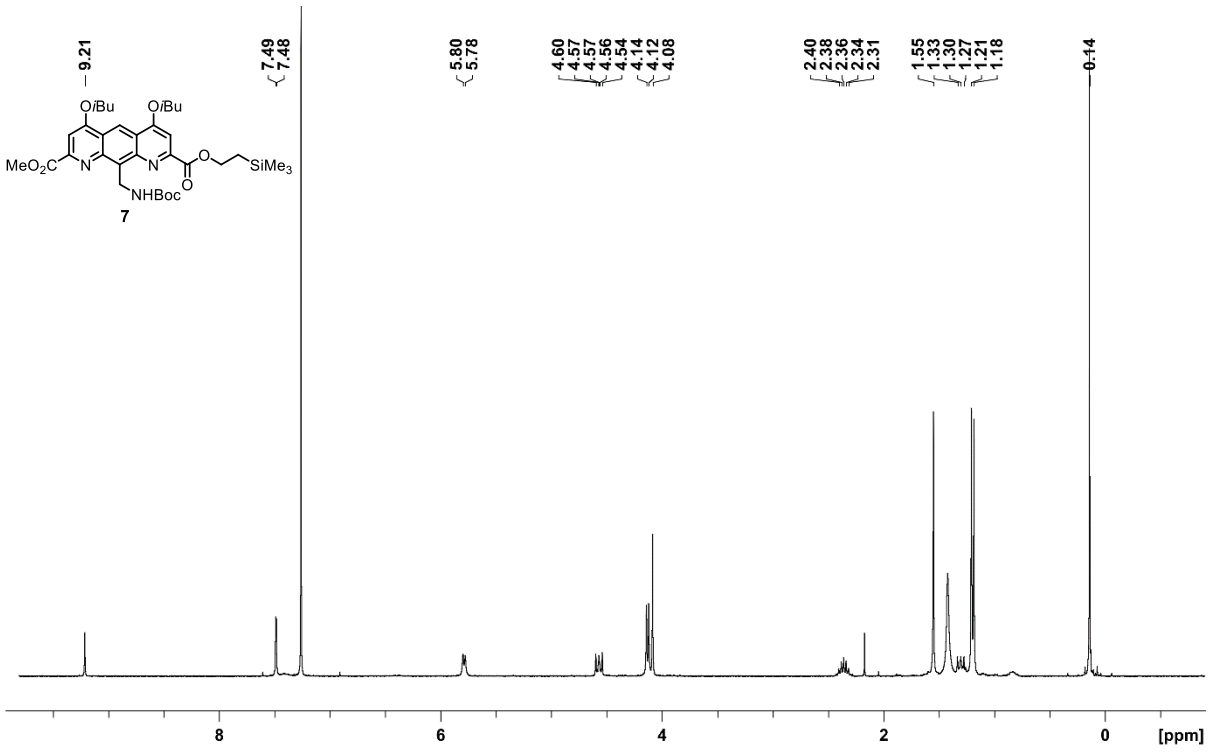
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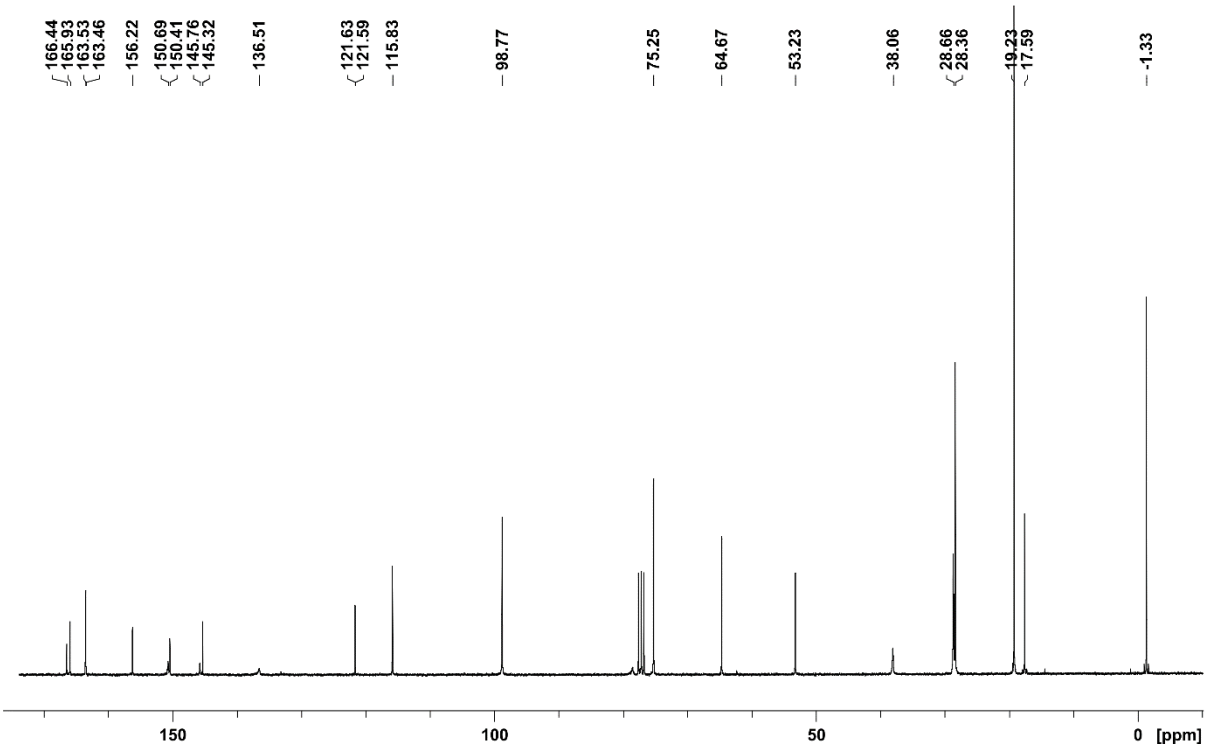
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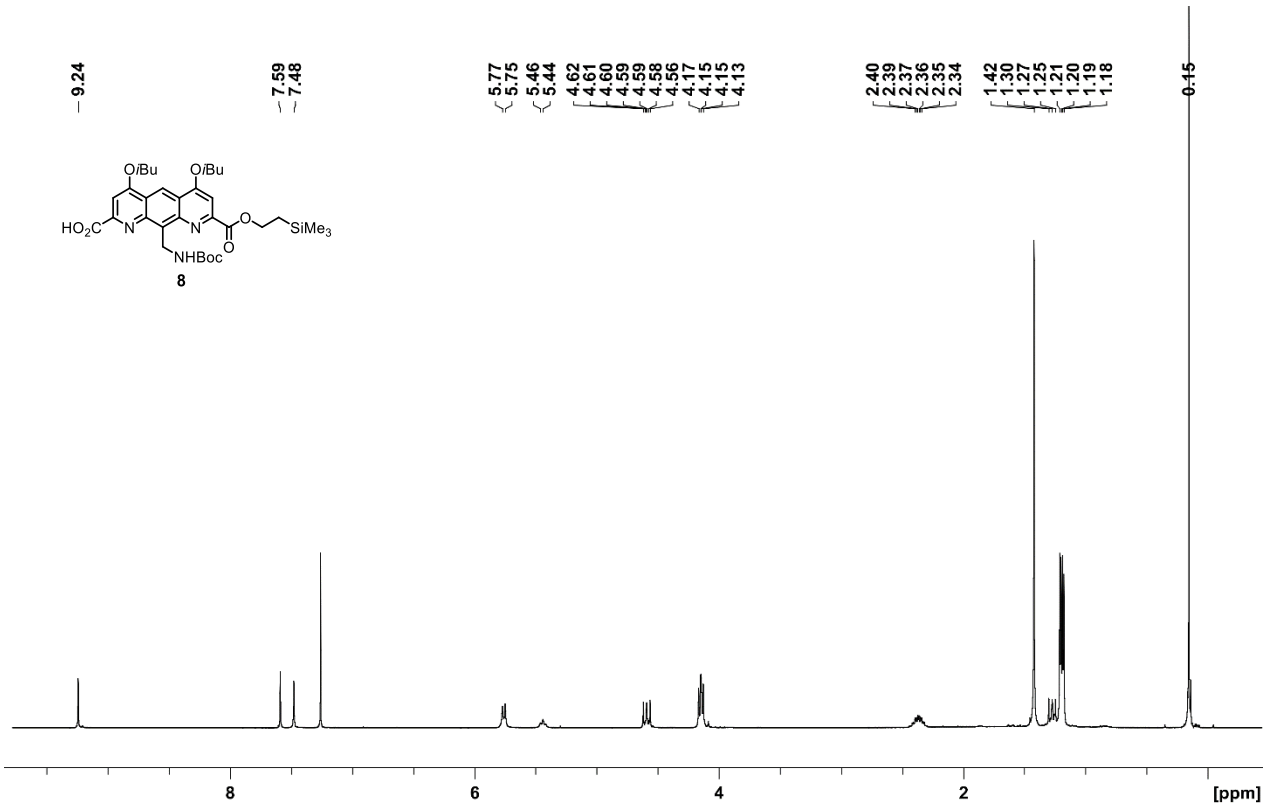
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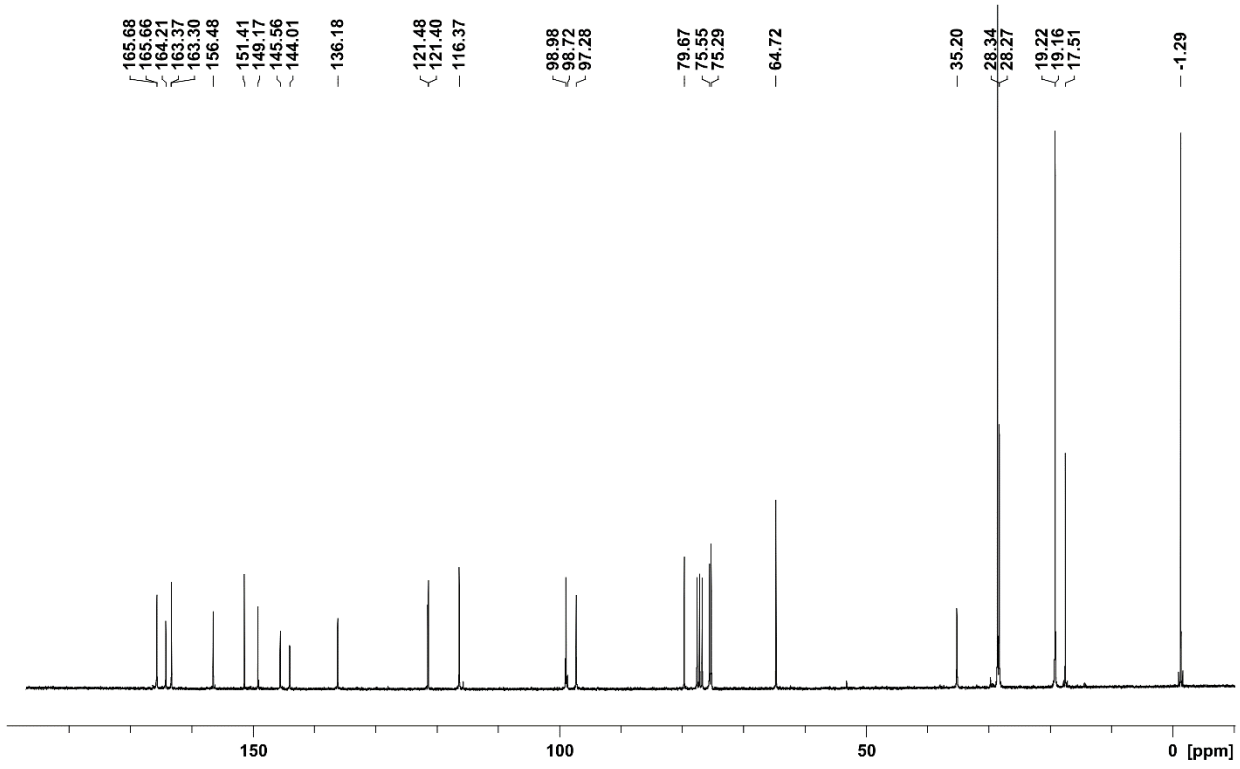
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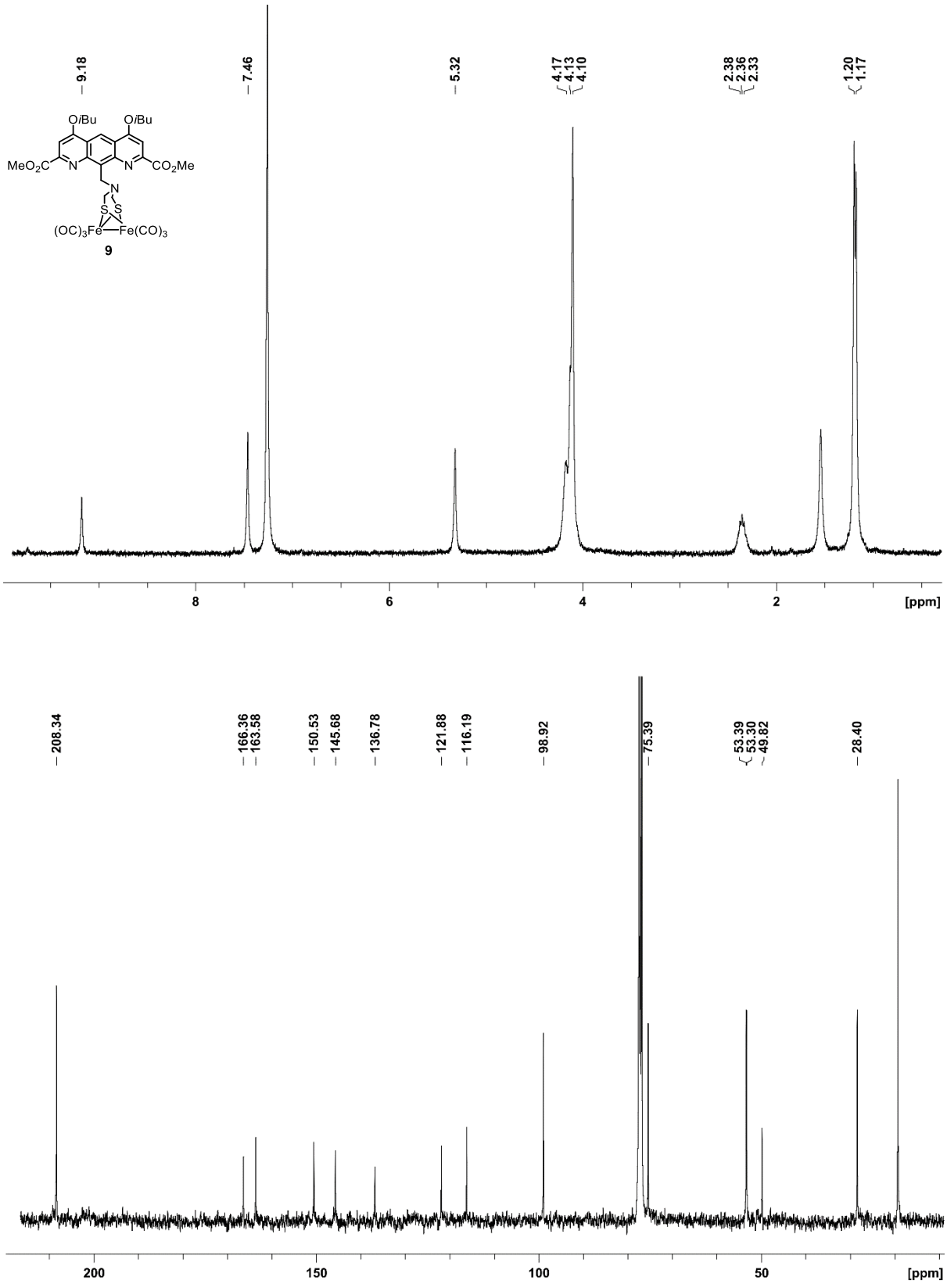
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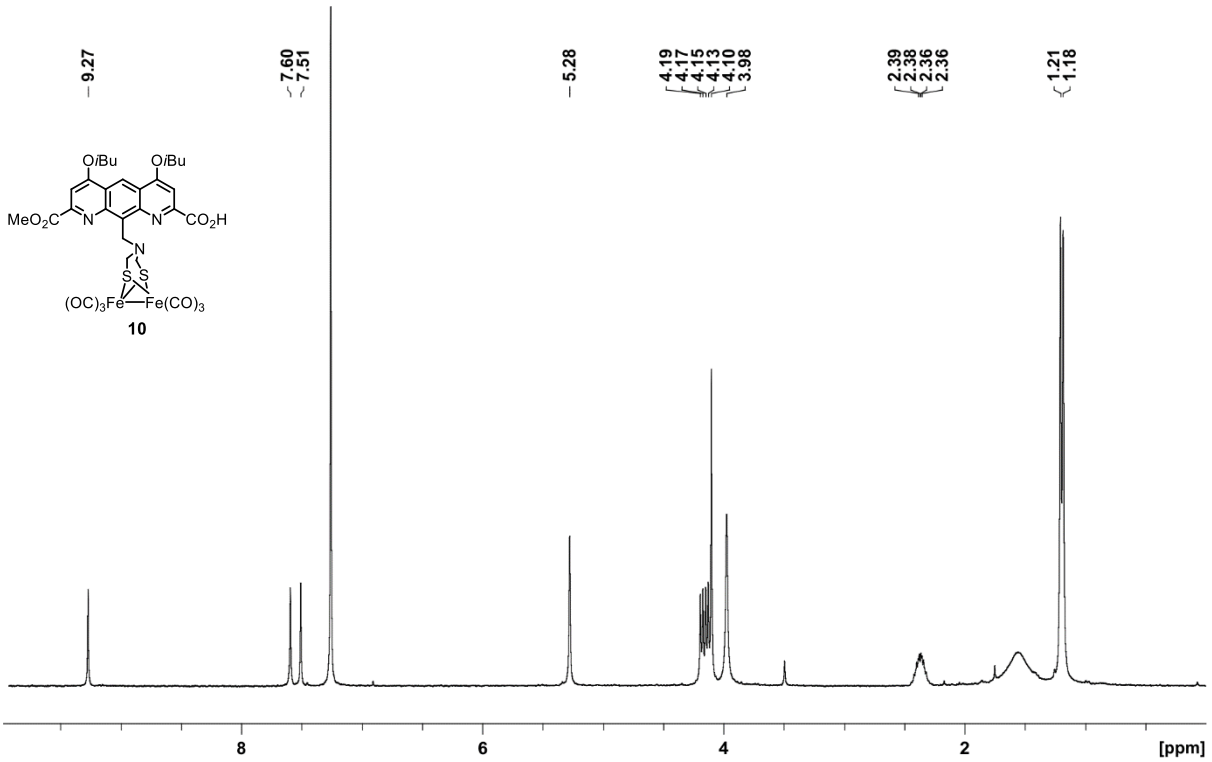
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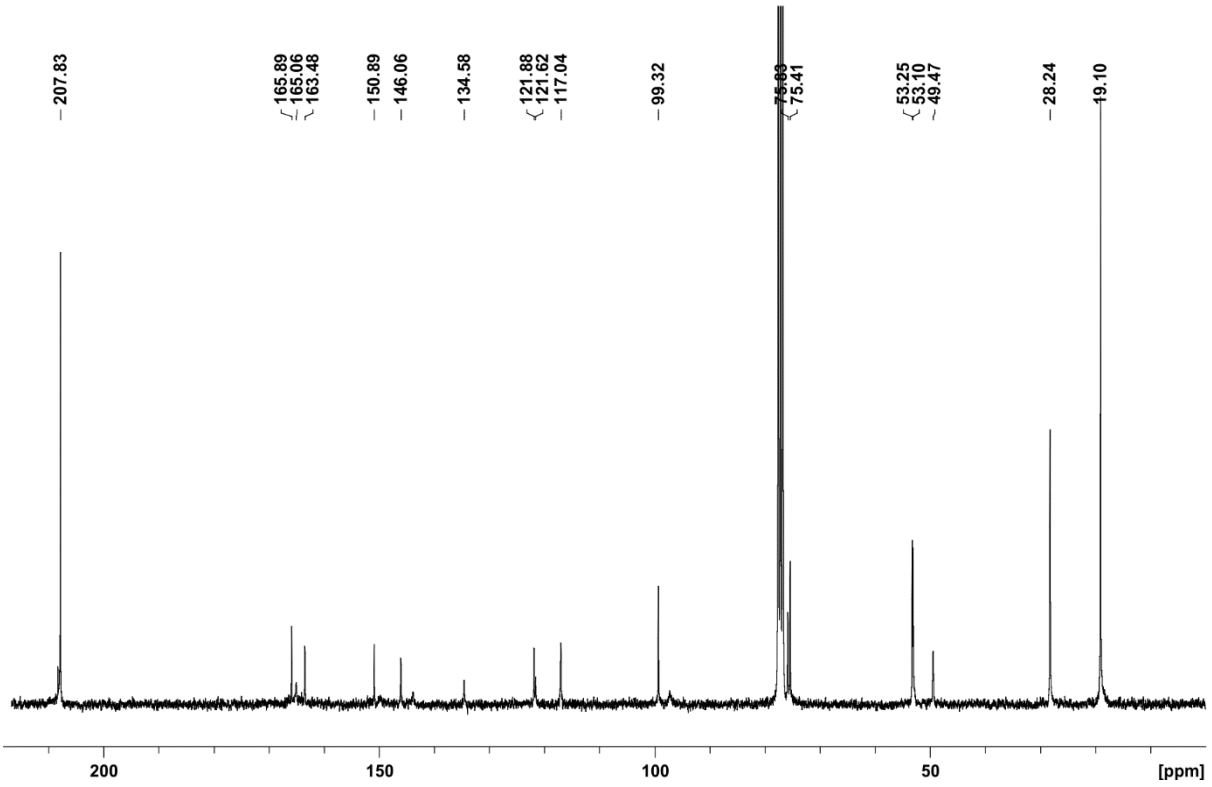
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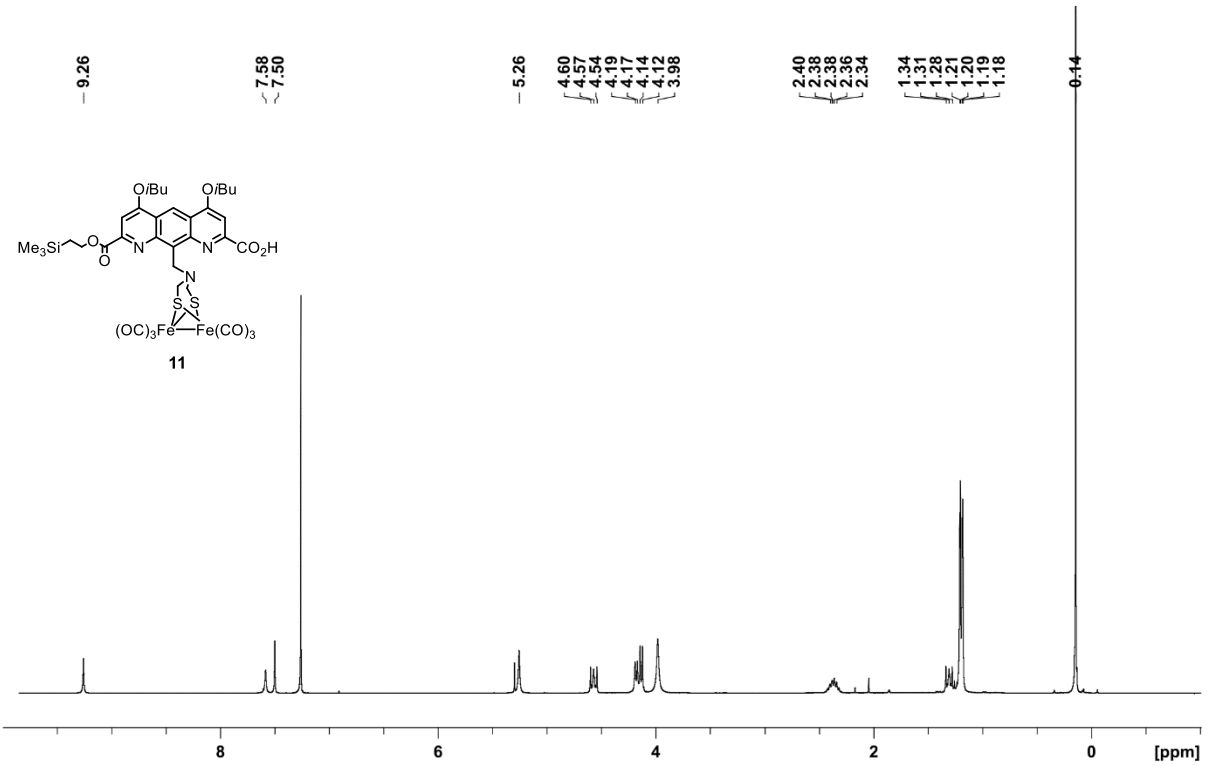
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2.38
2.38
2.36
2.34
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1.31
1.28
1.21
1.20
1.19
1.18
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CO2H
(OC)3Fe
Fe(CO)3
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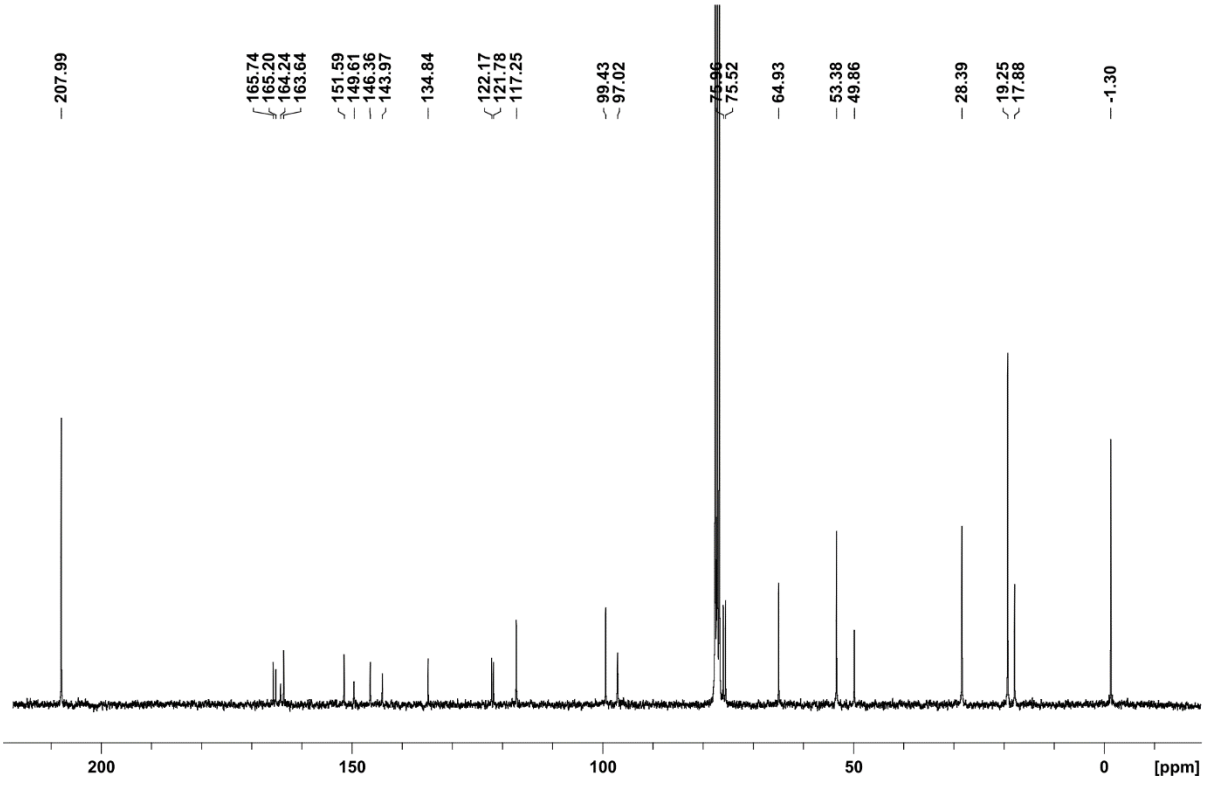
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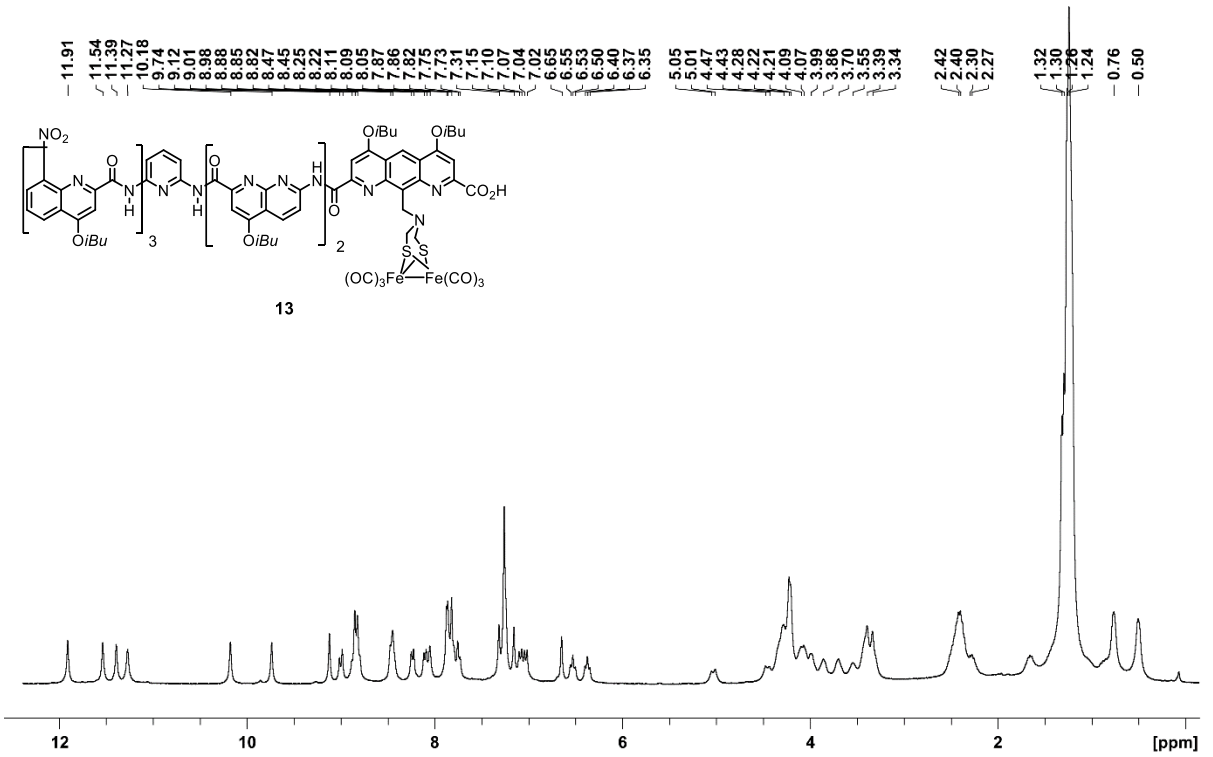
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8.22
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2.30
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1.30
1.26
1.24
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CO2H
(OC)3Fe
Fe(CO)3
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2
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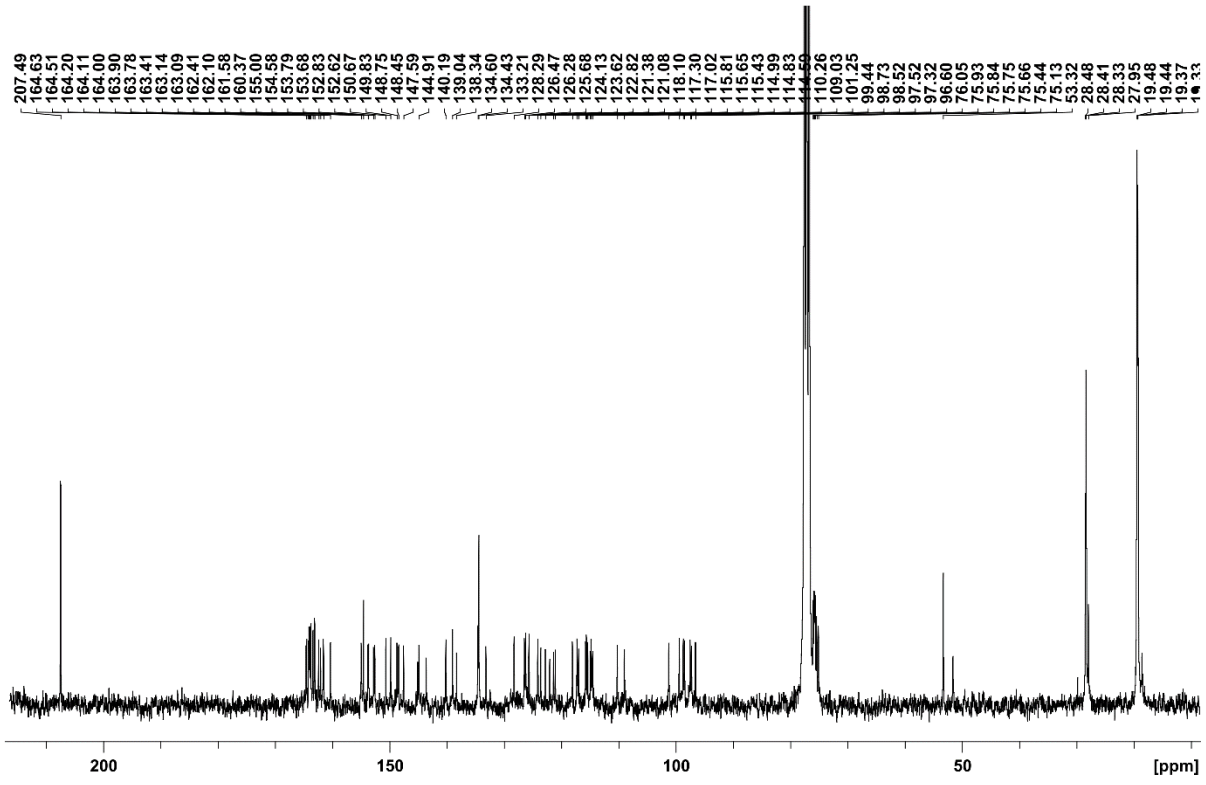
13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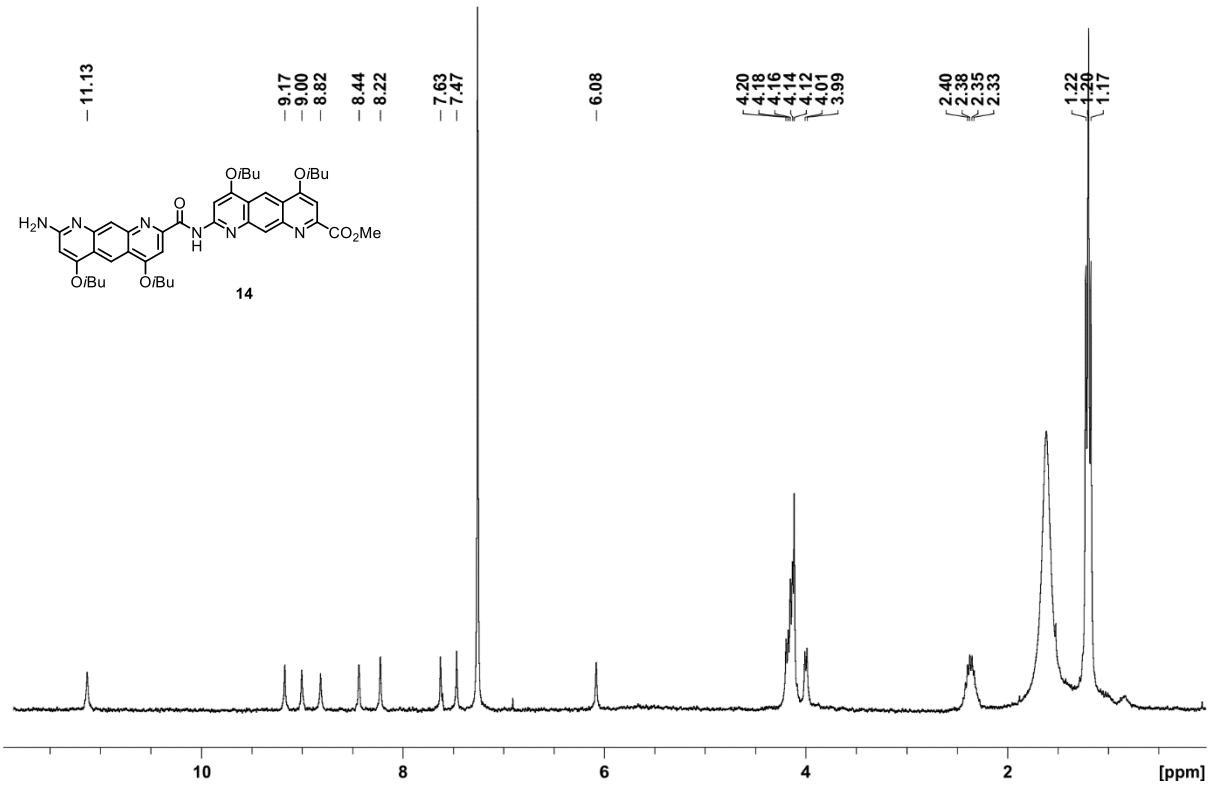
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4.18
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4.14
4.12
4.01
3.99
2.40
2.38
2.35
2.33
1.22
1.20
1.17
O*i*Bu
O*i*Bu
H_2N
N
N
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H
N
N
CO_2Me
O*i*Bu
O*i*Bu
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4
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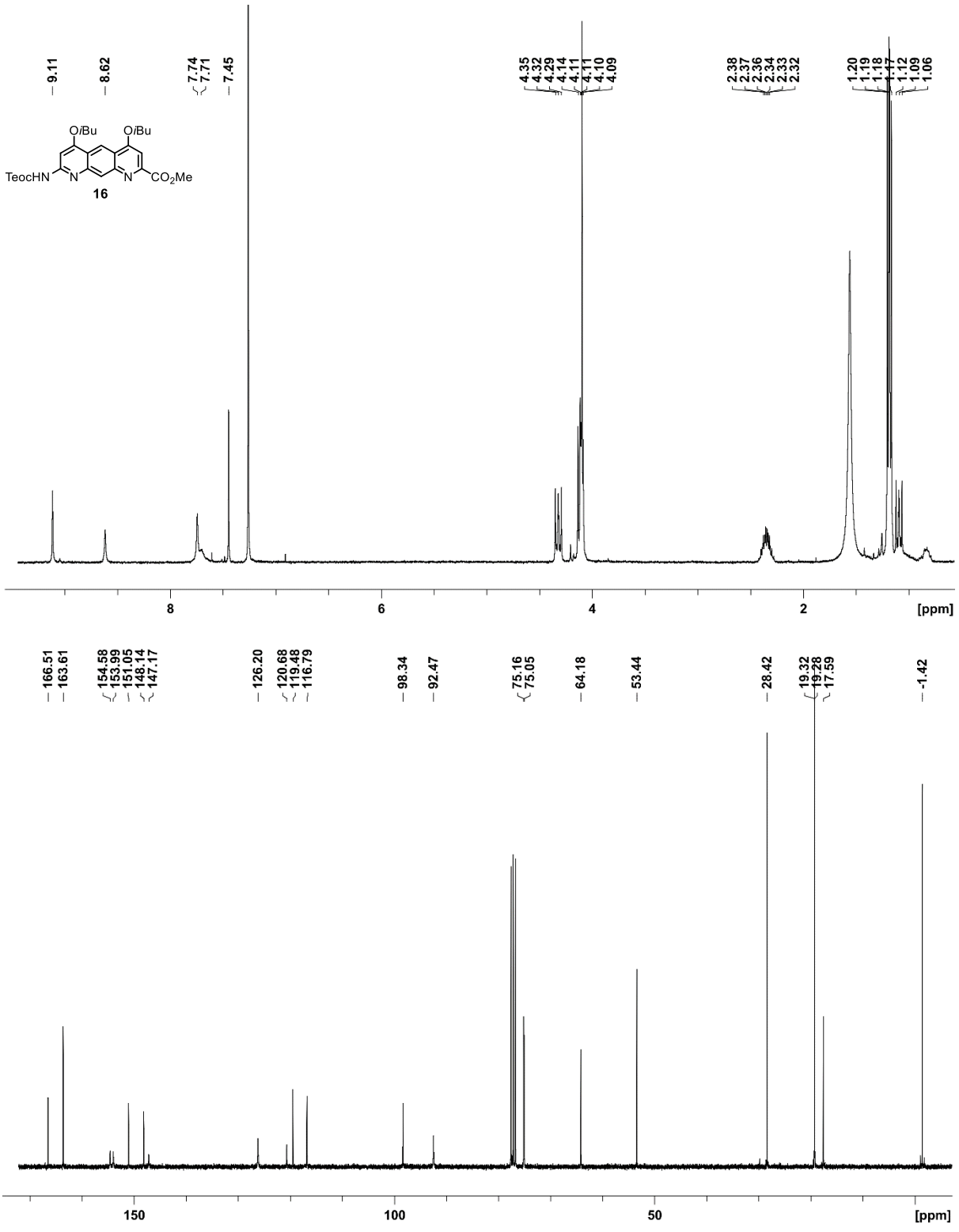
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4.11
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4.09
2.38
2.37
2.36
2.34
2.33
2.32
1.20
1.19
1.18
1.17
1.12
1.09
1.06
OiBu
OiBu
TeocHN
N
N
CO2Me
16
8
6
4
2
[ppm]
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153.99
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147.17
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120.68
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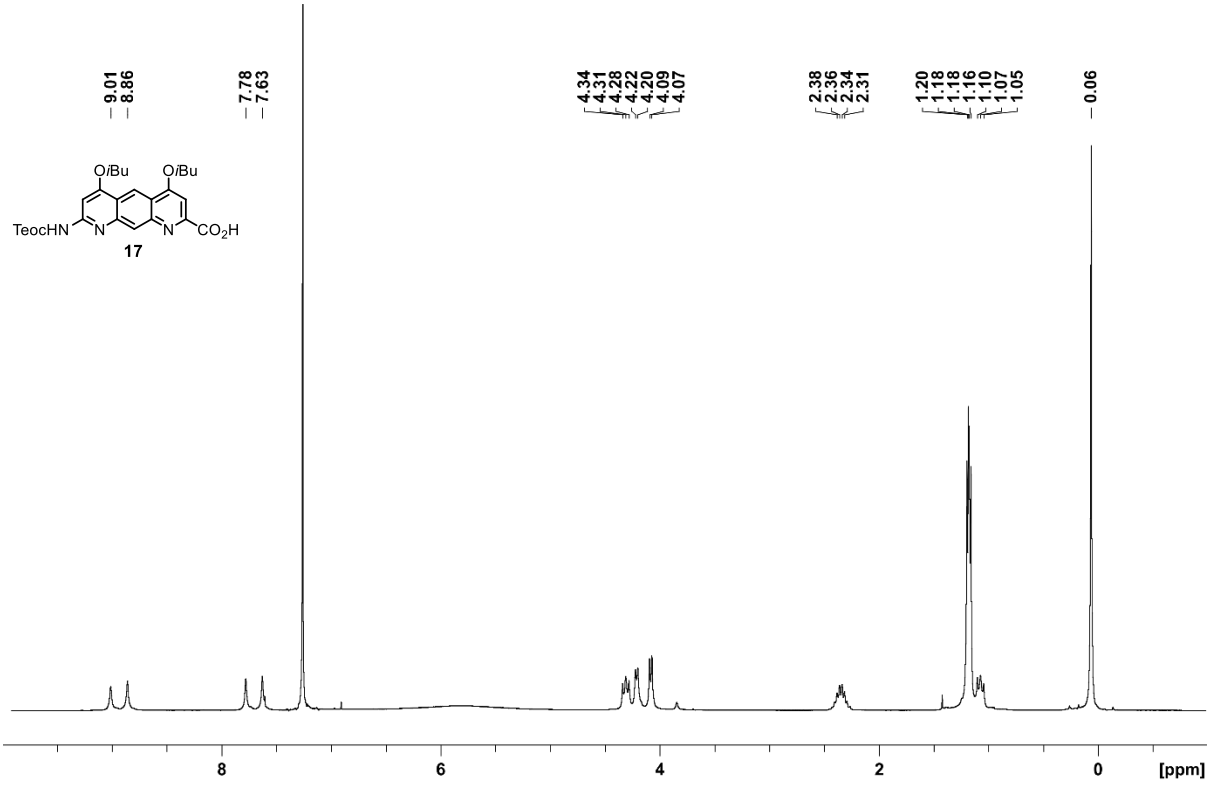
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4.09
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2.36
2.34
2.31
1.20
1.18
1.18
1.16
1.10
1.07
1.05
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O/Bu
O/Bu
TeocHN
N
N
CO2H
17
8
6
4
2
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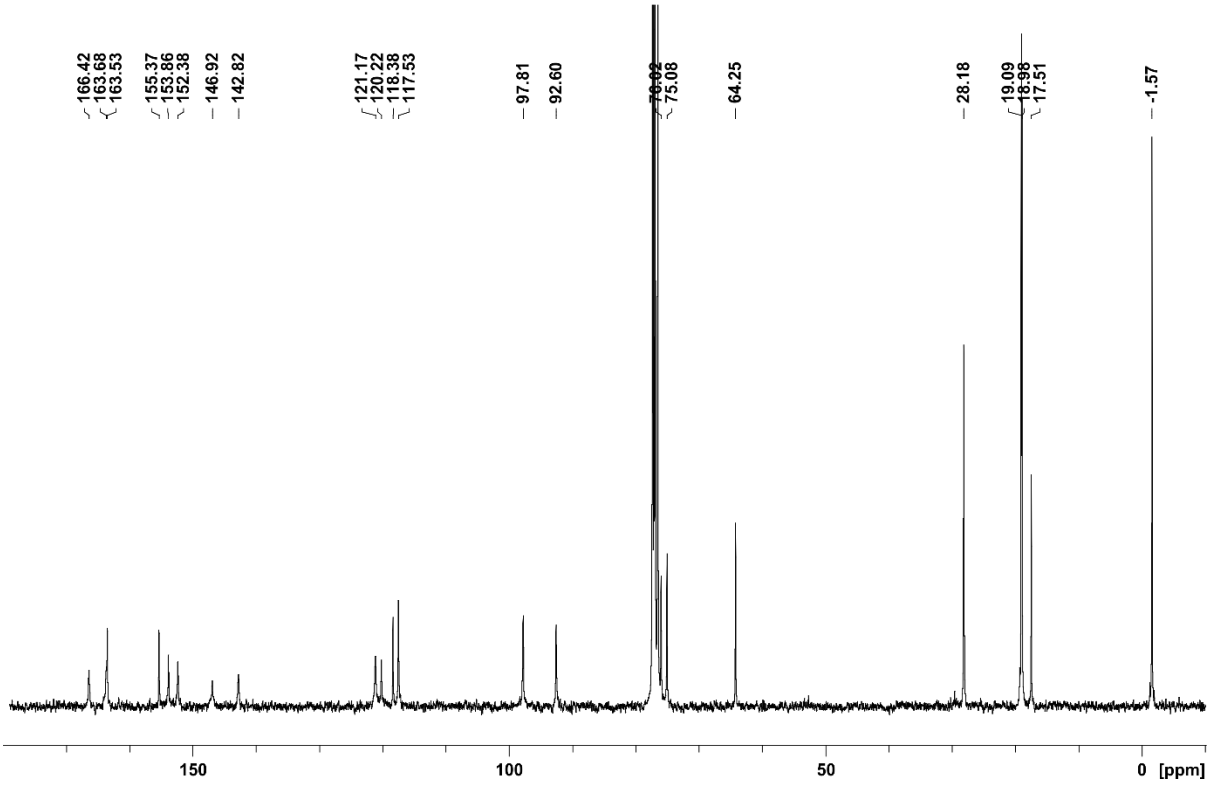
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18.98
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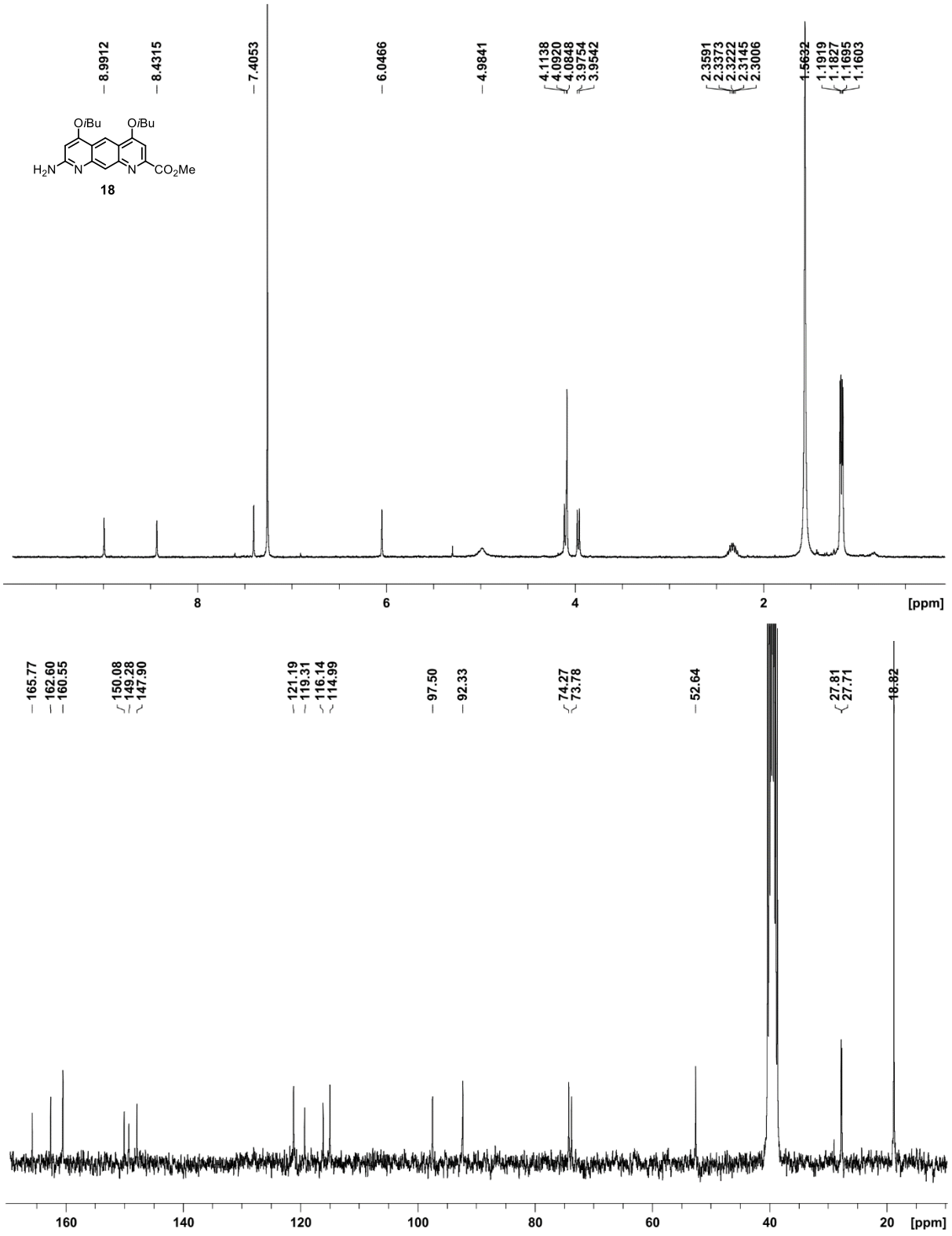
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2.3145
2.3006
1.5632
1.1919
1.1827
1.1695
1.1603
O/Bu
O/Bu
H2N
N
N
CO2Me
18
8
6
4
2
[ppm]
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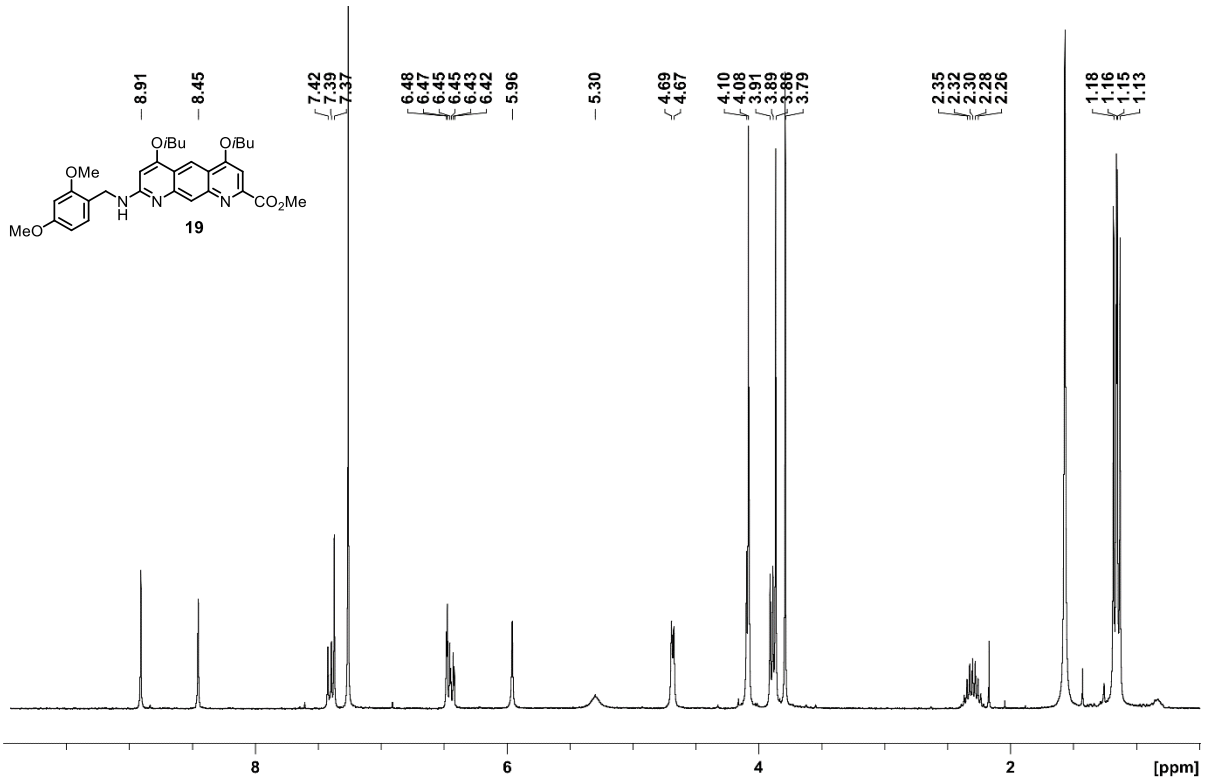
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5.30
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4.67
4.10
4.08
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3.89
3.86
3.79
2.35
2.32
2.30
2.28
2.26
1.18
1.16
1.15
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OiBu
OMe
MeO
N
H
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CO2Me
19
8
6
4
2
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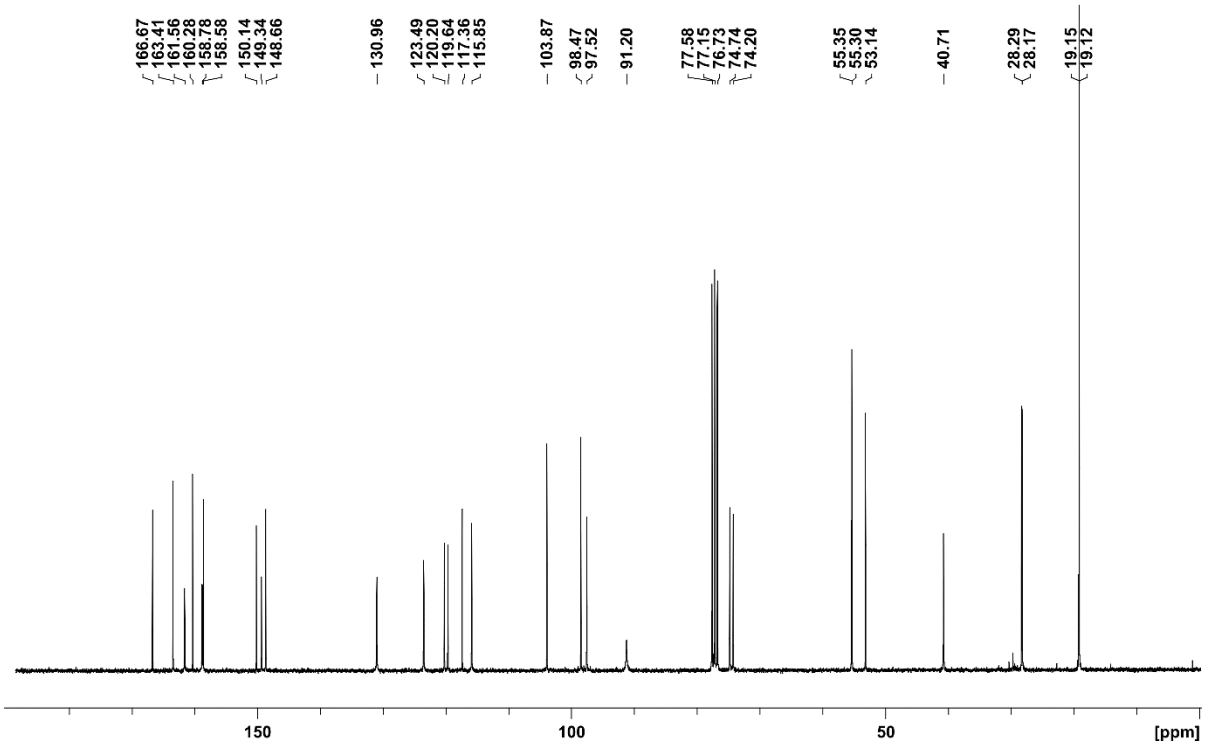
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91.20
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77.15
76.73
74.74
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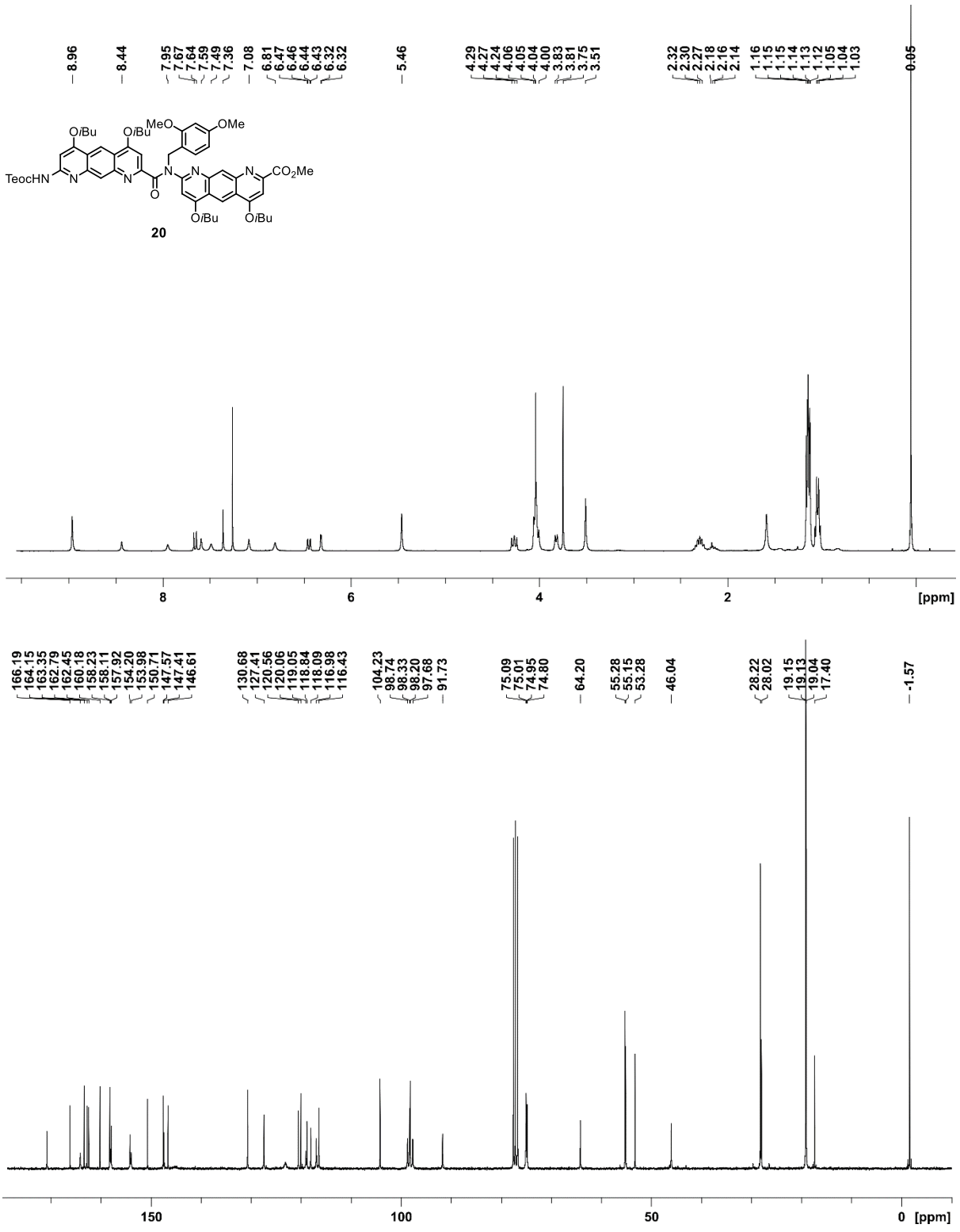
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7.08
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6.44
6.43
6.32
6.32
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2.27
2.18
2.16
2.14
1.16
1.15
1.15
1.14
1.13
1.12
1.05
1.04
1.03
0.05
OiBu
OiBu
MeO
OMe
TeocHN
N
N
N
N
N
CO2Me
O
OiBu
OiBu
20
8
6
4
2
[ppm]
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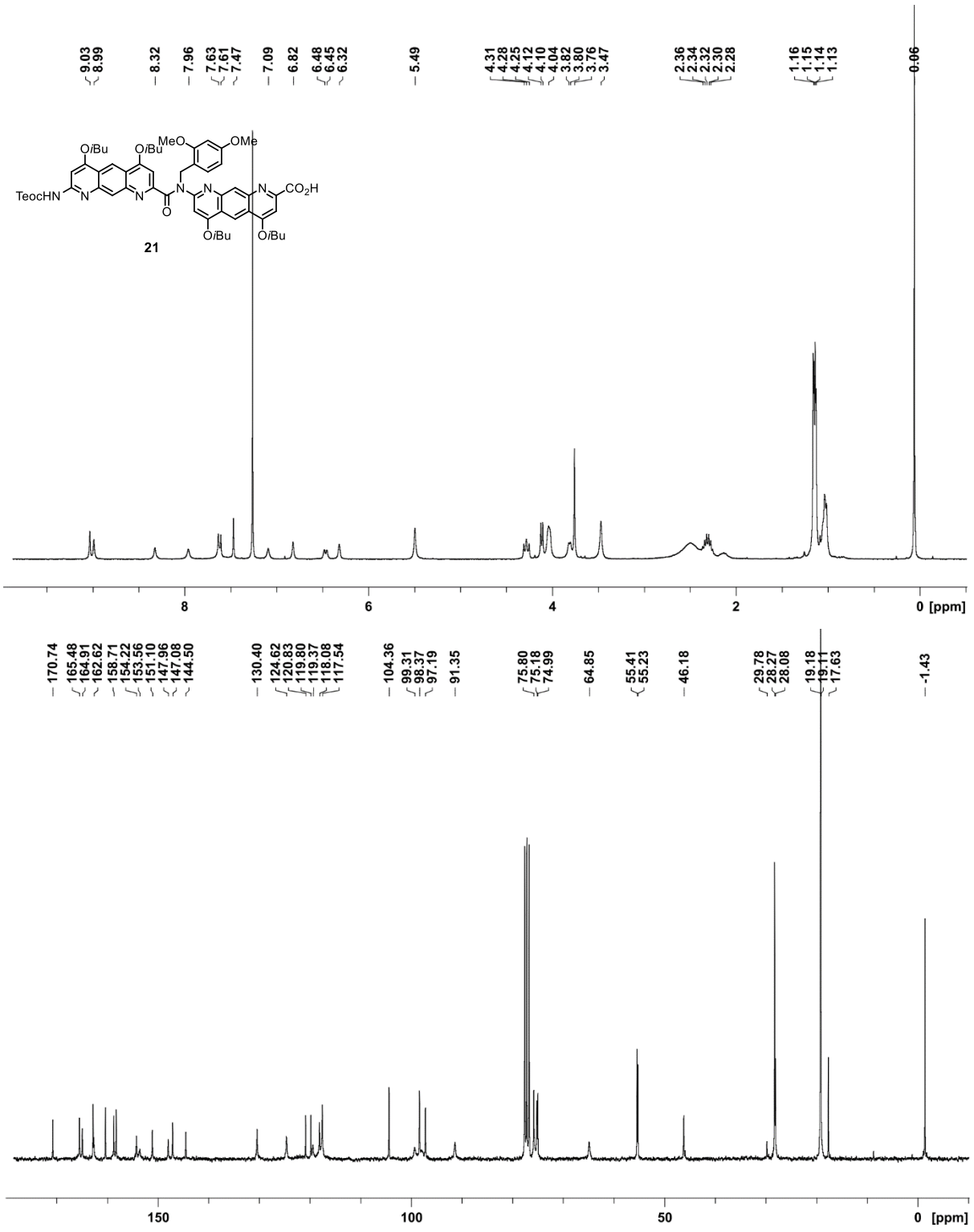
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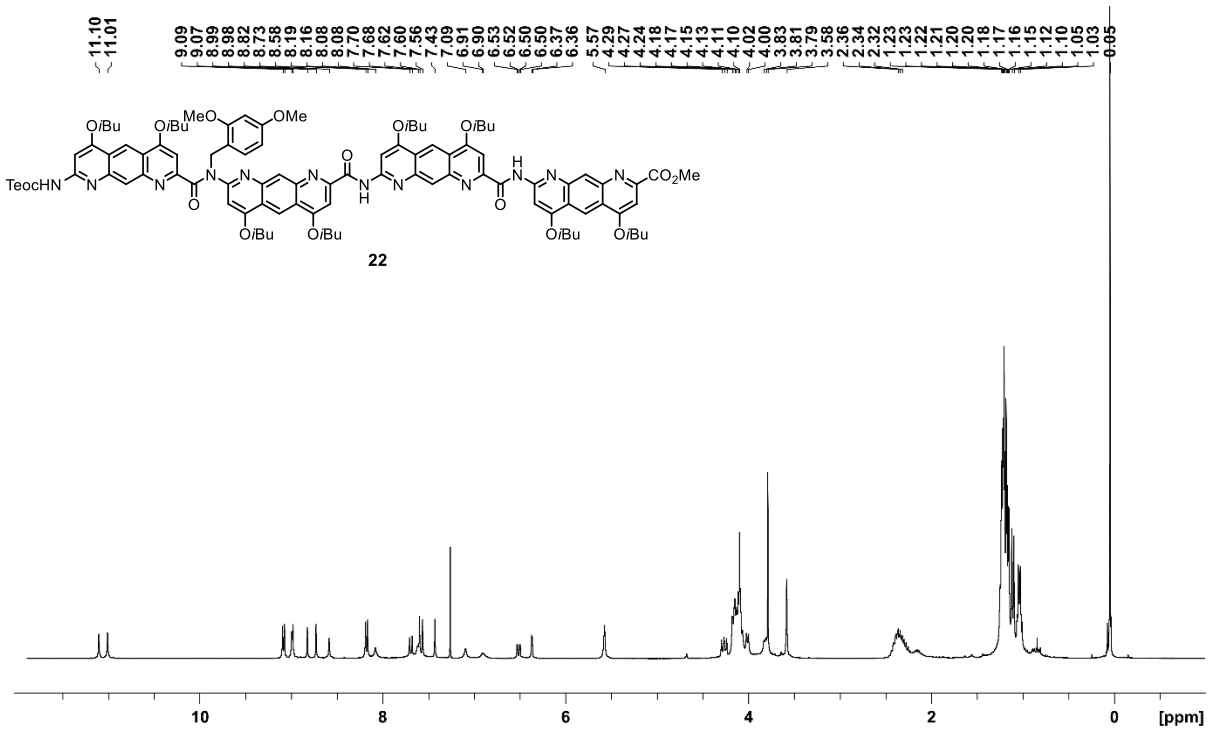
21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6.36
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4.02
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3.81
3.79
3.58
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2.34
2.32
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1.23
1.22
1.21
1.20
1.20
1.18
1.17
1.16
1.15
1.12
1.10
1.05
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OMe
OiBu
CO2Me
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10
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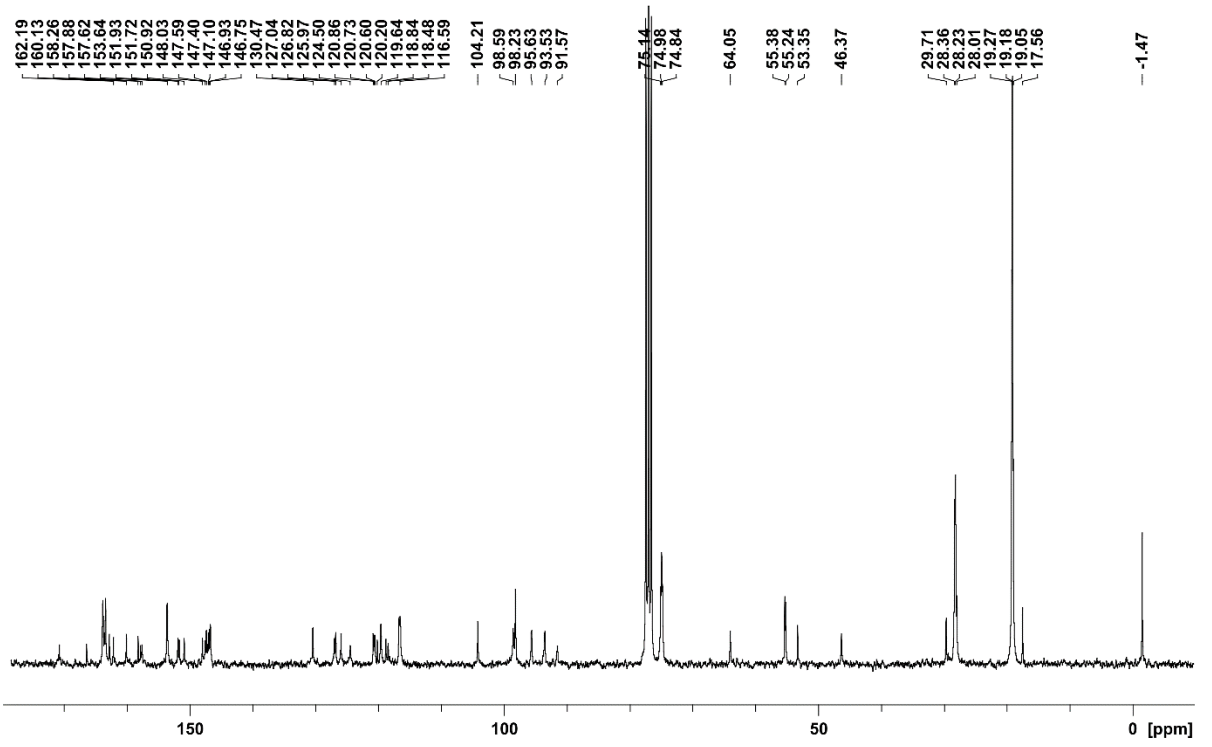
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74.84
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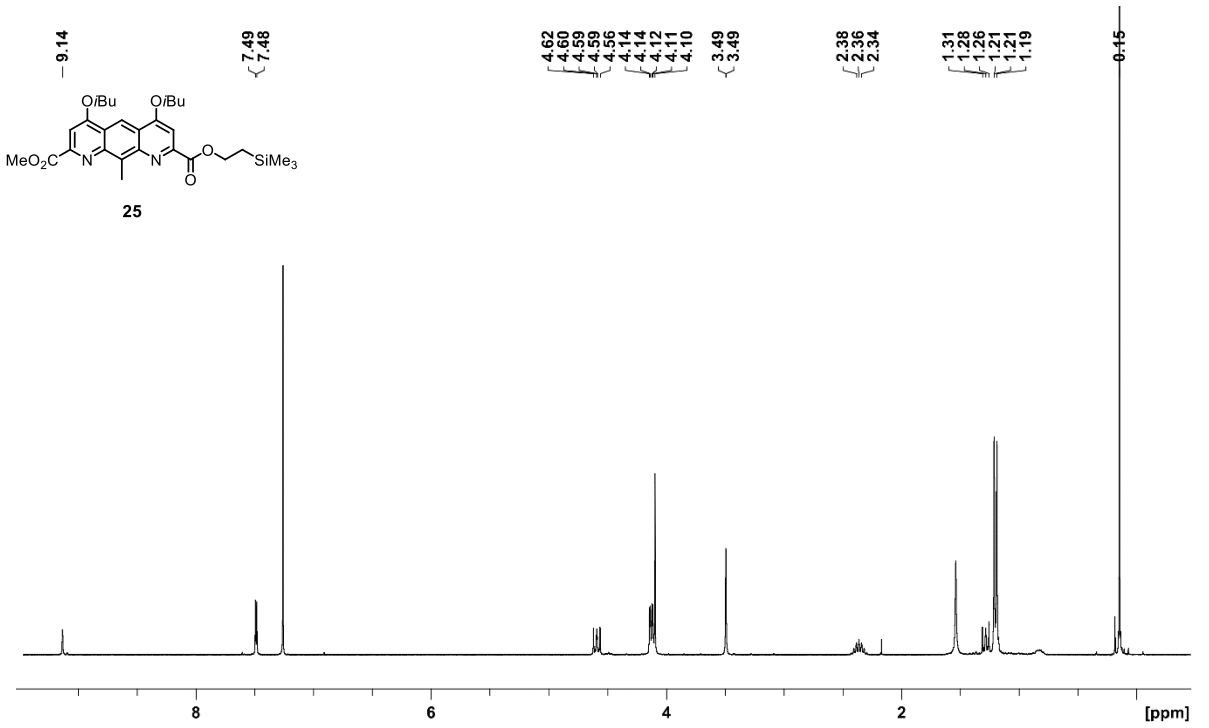
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4.10
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3.49
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2.36
2.34
1.31
1.28
1.26
1.21
1.21
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OiBu
MeO2C
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SiMe3
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4
2
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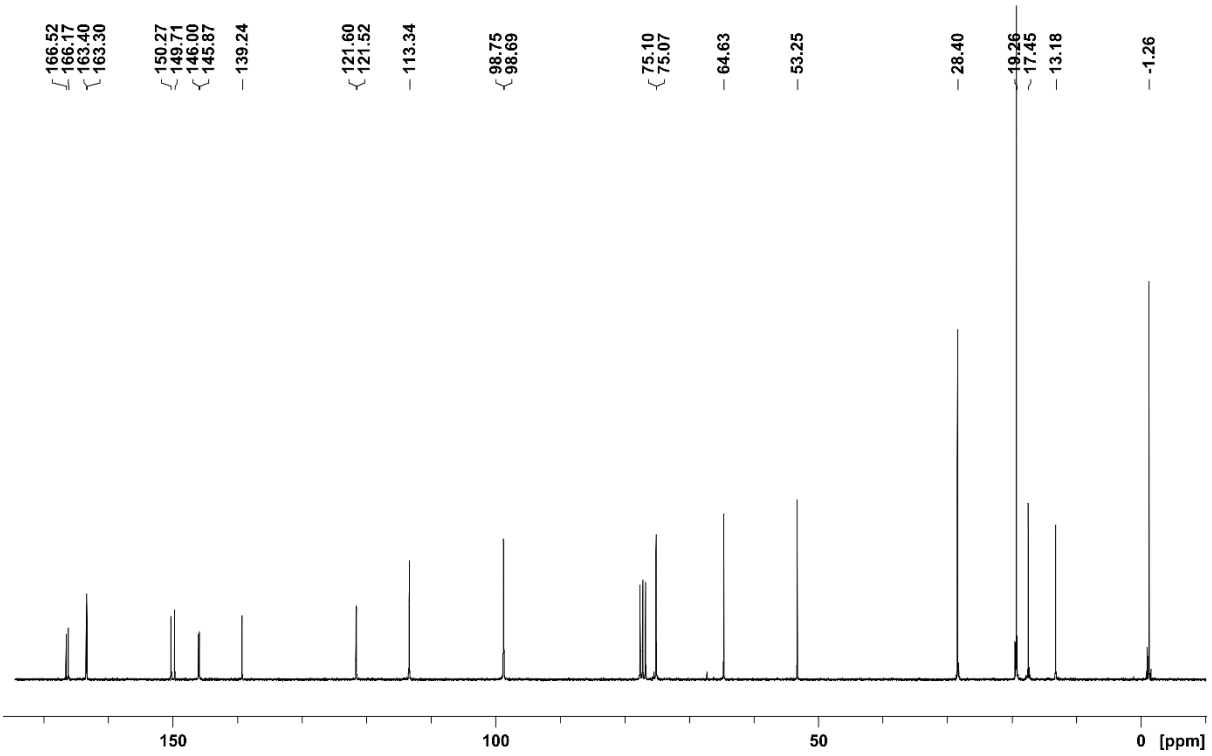
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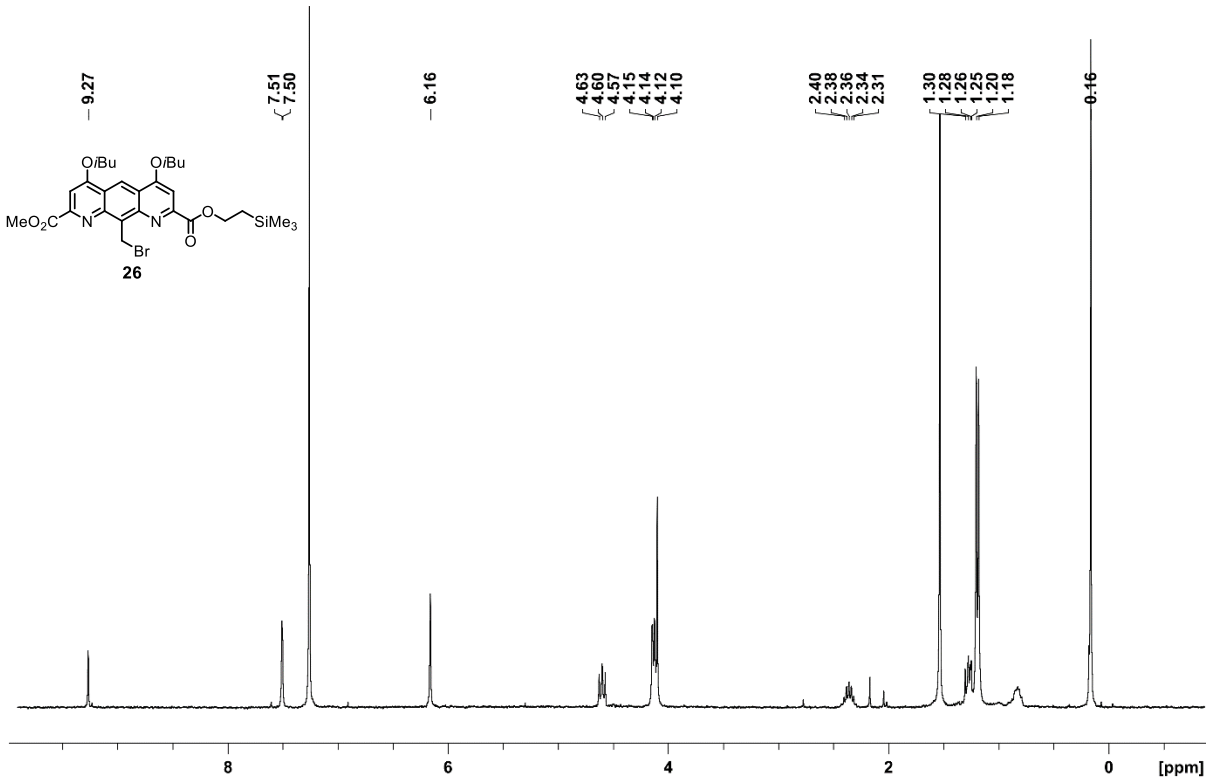
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4.12
4.10
2.40
2.38
2.36
2.34
2.31
1.30
1.28
1.26
1.25
1.20
1.18
0.16
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O/Bu
MeO2C
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Br
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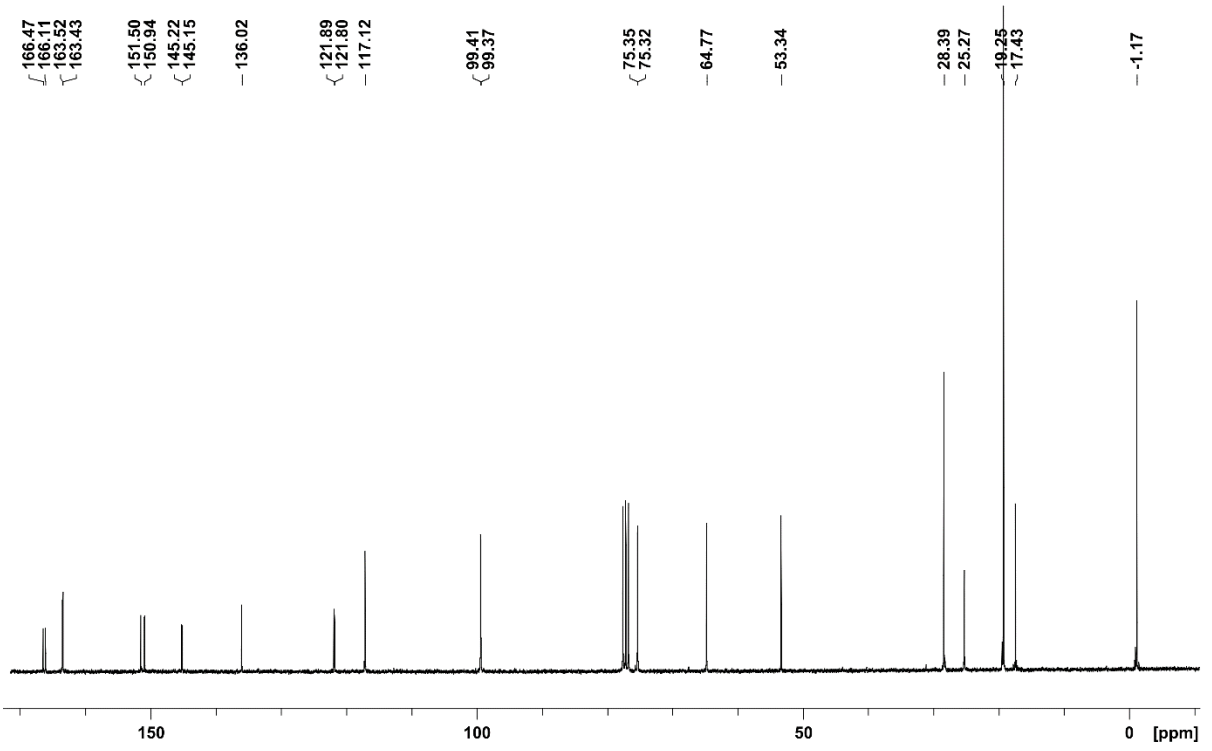
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99.37
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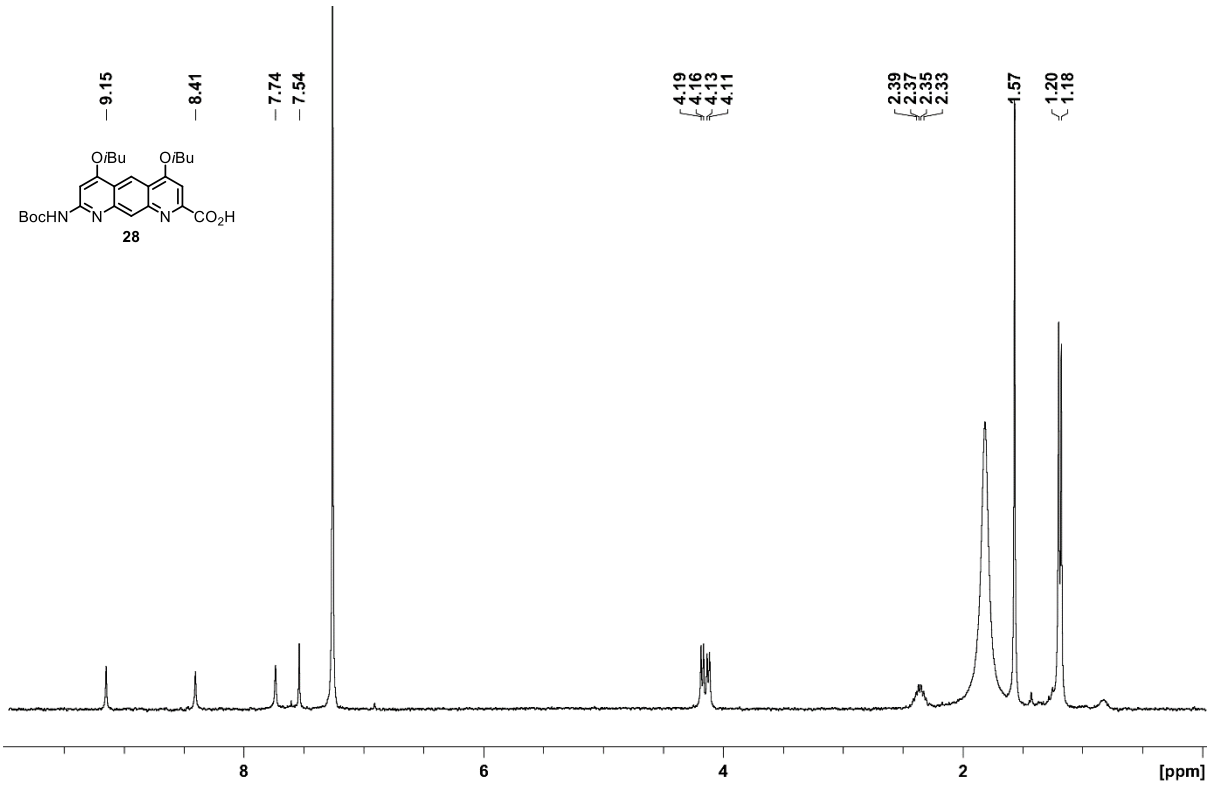
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4.16
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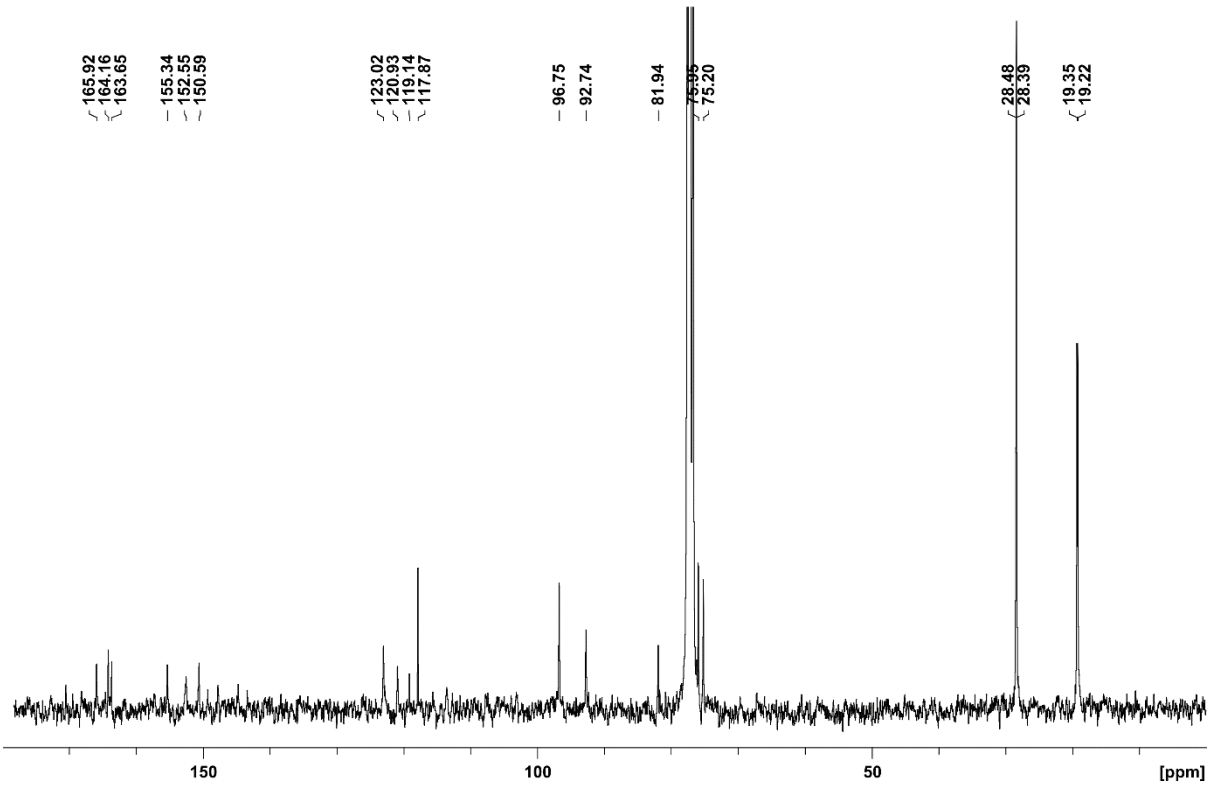
4.11
2.39
2.37
2.35
2.33
1.57
1.20
1.18
OiBu
OiBu
BocHN
N
N
CO2H
28
8
6
4
2
[ppm]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28.39
19.35
19.22
150
100
50
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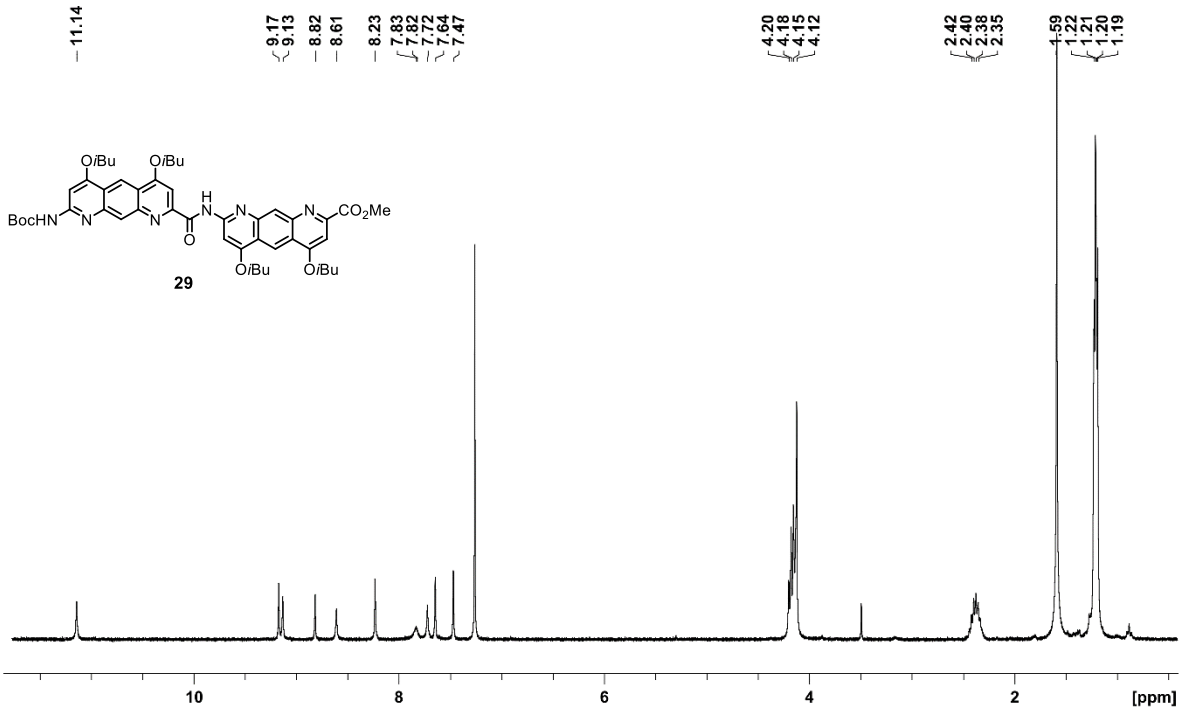
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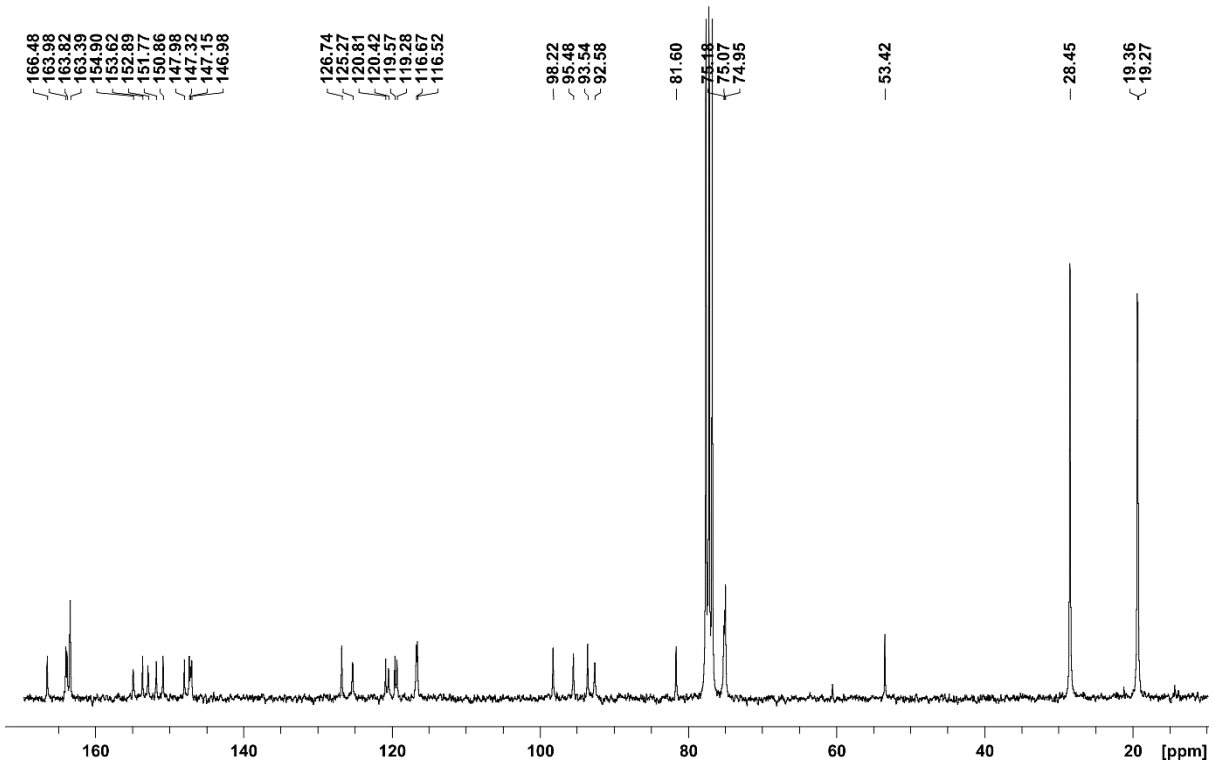
2.38
2.35
1.59
1.22
1.21
1.20
1.19
O/Bu
O/Bu
BocHN
H
N
CO2Me
O
O/Bu
O/Bu
29
10
8
6
4
2
[ppm]


166.48
163.98
163.82
163.39
154.90
153.62
152.89
151.77
150.86
147.98
147.32
147.15
146.98
126.74
125.27
120.81
120.42
119.57
119.28
116.67
116.52
98.22
95.48
93.54
92.58
81.60
75.18
75.07
74.95
53.42
28.45
19.36
19.27
160
140
120
100
80
60
40
20
[ppm]

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) q3pn2afe_a_sq

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: q3pn2afe_a_sq

```
Bond precision:  C-C = 0.0264 A          Wavelength=1.54178

Cell:            a=42.379(9)     b=22.277(5)       c=31.801(6)
                 alpha=90        beta=98.36(3)     gamma=90
Temperature:     130 K
```

	Calculated	Reported
Volume	29704(11)	29704(11)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C104 H102 Fe2 N19 O23 S2, 3(C H Cl3) [+ solvent]	C104 H102 Fe2 N19 O23 S2, 3(C H Cl3)
Sum formula	C107 H105 Cl9 Fe2 N19 O23 S2 [+ solvent]	C107 H105 Cl9 Fe2 N19 O23 S2
Mr	2519.98	2519.96
Dx,g cm-3	1.127	1.127
Z	8	8
Mu (mm-1)	3.826	3.826
F000	10408.0	10408.0
F000’	10449.66	
h,k,lmax	40,21,30	40,21,30
Nref	13439	13285
Tmin,Tmax	0.716,0.682	0.283,1.000
Tmin’	0.650	

```
Correction method= # Reported T Limits: Tmin=0.283 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.989          Theta(max)= 47.238

R(reflections)= 0.1284( 6926)     wR2(reflections)= 0.3765( 13285)

S = 1.132                 Npar= 1474
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level A

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
Calculated sin(theta_max)/wavelength = 0.4762
PLAT234_ALERT_4_A Large Hirshfeld Difference C8 --C04G . 0.37 Ang.
PLAT234_ALERT_4_A Large Hirshfeld Difference C01R --C02F . 0.32 Ang.

Alert level B

PLAT084_ALERT_3_B High wR2 Value (i.e. > 0.25) ..... 0.38 Report
PLAT234_ALERT_4_B Large Hirshfeld Difference O00H --C01T . 0.29 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference O00K --C024 . 0.28 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference N015 --C02K . 0.26 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference N01G --C01F . 0.27 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference C01W --C02W . 0.29 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference C01Y --C03I . 0.26 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference C02B --C02E . 0.28 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference C02C --C031 . 0.30 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference C02V --C038 . 0.27 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference C02Y --C03S . 0.26 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference C03B --C03P . 0.28 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference C03E --C04B . 0.26 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference C03F --C045 . 0.28 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference C03K --C03T . 0.26 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference C03X --C03Z . 0.26 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference C048 --C04J . 0.30 Ang.
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of N01G Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of C04G Check
PLAT260_ALERT_2_B Large Average Ueq of Residue Including Cl3 0.415 Check
PLAT260_ALERT_2_B Large Average Ueq of Residue Including Cl4 0.370 Check
PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.02641 Ang.
PLAT369_ALERT_2_B Long C(sp2)-C(sp2) Bond C01O - C021 . 1.59 Ang.
PLAT369_ALERT_2_B Long C(sp2)-C(sp2) Bond C02I - C02Q . 1.57 Ang.

Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.
Absorption correction given as multi-scan
CRYSC01_ALERT_1_C No recognised colour has been given for crystal colour.
PLAT082_ALERT_2_C High R1 Value ..... 0.13 Report
PLAT088_ALERT_3_C Poor Data / Parameter Ratio ..... 9.01 Note
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.5 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for O00B --C023 . 5.1 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for N00Q --C01U . 5.2 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for N015 --C022 . 6.6 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for C024 --C02V . 5.7 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for C02F --C03B . 5.5 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference Fe01 --C02O . 0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Fe01 --C02R . 0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Fe02 --C032 . 0.24 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O00A --C026 . 0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O00C --C02X . 0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O00I --C02L . 0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O00I --C03W . 0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O00O --C02E . 0.18 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference O00W --C02R . 0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O014 --C02J . 0.24 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O017 --C025 . 0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O01C --C02Y . 0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O01E --C032 . 0.23 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O01Q --C042 . 0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N00F --C01D . 0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N00F --C01H . 0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N00R --C023 . 0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N00T --C02H . 0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N00X --C01R . 0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N00X --C02B . 0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N011 --C029 . 0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N012 --C02E . 0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N012 --C02G . 0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N013 --C02D . 0.25 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N013 --C02Z . 0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N01A --C024 . 0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N01G --C01D . 0.23 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N01G --C036 . 0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N01K --C029 . 0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N01K --C02I . 0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N01N --C02U . 0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C01F --C01J . 0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C01H --C023 . 0.25 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C01I --C01P . 0.23 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C01J --C020 . 0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C01J --C026 . 0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C01O --C021 . 0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C01R --C02A . 0.24 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C01U --C02N . 0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C02I --C02Q . 0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C033 --C03O . 0.25 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O01C Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C01P Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C01T Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C03P Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C03R Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C03S Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C03T Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C03X Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C03Z Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N00U Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C01D Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C01F Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C01H Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C02D Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C02K Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C02T Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C02Y Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C036 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C037 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C03C Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C03E Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C03M Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C03Q Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C03W Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C03Y Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C04A Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C040 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C04P Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C04K Check

```
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      Fe01      0.153 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      Cl05      0.184 Check
PLAT336_ALERT_2_C Long Bond Distance for ..... C04K     -Cl4           1.900 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C022     - C02T     .      1.55 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      9.680 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      3.503 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.113 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.476        154 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .          1 Check
PLAT923_ALERT_1_C S    Values in the CIF and FCF Differ by .......      0.013 Check
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..          1 Check
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          4 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          5 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          6 Report
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.20 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          3 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records          1 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Fe01     --C01T     .        6.8 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Fe02     --C025     .        5.9 s.u.
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C01R     -C02F          0.15 Ang.
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C022     -C03A          0.25 Ang.
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C02G     -C03H          0.18 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O00J     ..C04P           3.00 Ang.
                                                     x,y,z  =      1_555 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact Cl4      ..Cl4            3.19 Ang.
                                                1-x,y,3/2-z  =      2_656 Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........          ! Info
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........        256 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         27 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed           ! Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          2 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          3 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        3.5 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
```

```
  3 ALERT level A = Most likely a serious problem - resolve or explain
 24 ALERT level B = A potentially serious problem, consider carefully
 91 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 22 ALERT level G = General information/check it is not something unexpected

  3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 55 ALERT type 2 Indicator that the structure model may be wrong or deficient
 14 ALERT type 3 Indicator that the structure quality may be low
 67 ALERT type 4 Improvement, methodology, query or suggestion
  1 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

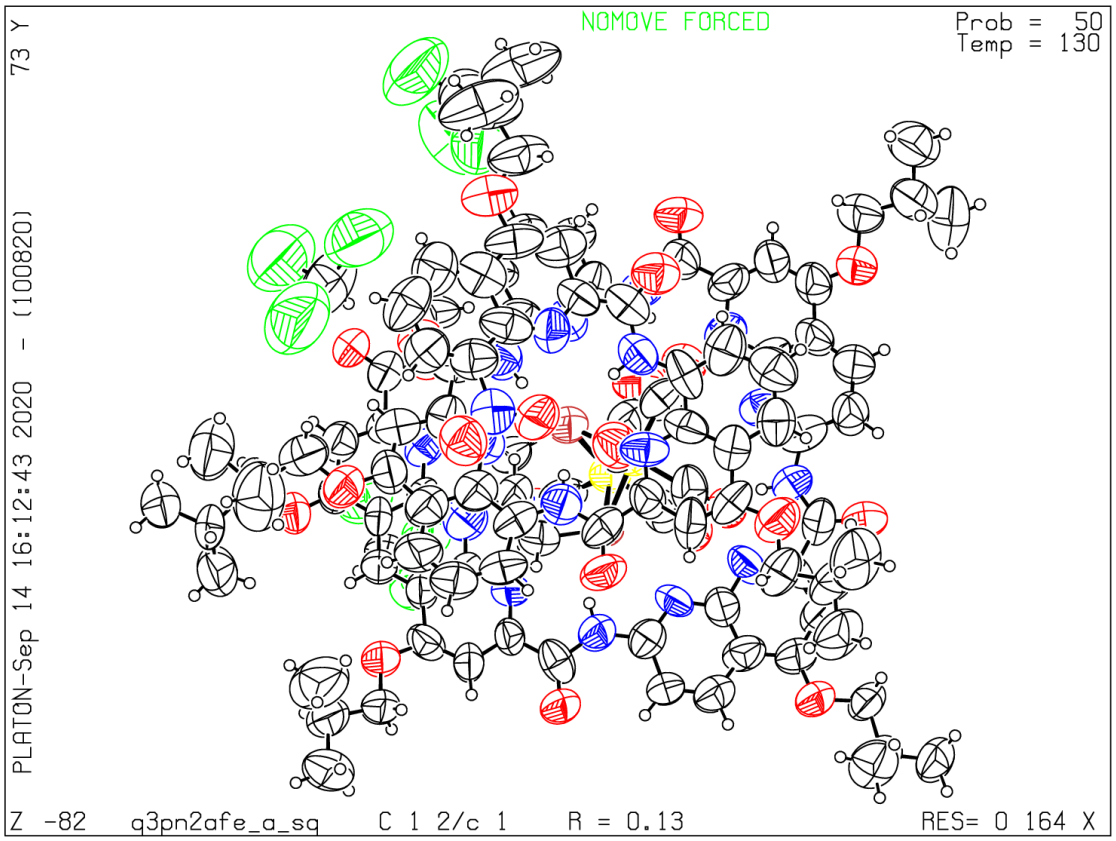
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 10/08/2020; check.def file version of 06/08/2020

Datablock q3pn2afe_a_sq - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ah2fip_a_sq_sq

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: ah2fip_a_sq_sq

```
Bond precision:  C-C = 0.0132 A          Wavelength=0.81000

Cell:           a=17.679(4)       b=22.049(4)      c=25.574(5)
                alpha=72.80(3)    beta=73.10(3)    gamma=79.74(3)
Temperature:    100 K
```

	Calculated	Reported
Volume	9065(4)	9066(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C147 H149 Fe2 N24 O29 S2, C H Cl3 [+ solvent]	?
Sum formula	C148 H150 Cl3 Fe2 N24 O29 S2 [+ solvent]	C148 H150 Cl3 Fe2 N24 O29 S2
Mr	3011.10	3011.08
Dx,g cm-3	1.103	1.103
Z	2	2
Mu (mm-1)	0.413	0.413
F000	3146.0	3146.0
F000′	3151.13	
h,k,lmax	19,24,28	19,24,28
Nref	26911	24578
Tmin,Tmax	0.960,0.960	
Tmin′	0.960	

```
Correction method= Not given

Data completeness= 0.913          Theta(max)= 27.067

R(reflections)= 0.1129( 15839)    wR2(reflections)= 0.3608( 24578)

S = 1.367                 Npar= 1917
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level A

SHFSU01_ALERT_2_A The absolute value of parameter shift to su ratio > 0.20
Absolute value of the parameter shift to su ratio given 0.622
Additional refinement cycles may be required.

```
PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low .      0.913 Why?
PLAT080_ALERT_2_A Maximum Shift/Error ..........................       0.62 Why ?
PLAT412_ALERT_2_A Short Intra XH3 .. XHn     H48A     ..H04K     .       1.65 Ang.
                                             x,y,z  =      1_555 Check
PLAT412_ALERT_2_A Short Intra XH3 .. XHn     H48B     ..H04X     .       1.38 Ang.
                                             x,y,z  =      1_555 Check
PLAT412_ALERT_2_A Short Intra XH3 .. XHn     H053     ..Hb       .       1.69 Ang.
                                             x,y,z  =      1_555 Check
```

Alert level B

THETM01_ALERT_3_B The value of sine(theta_max)/wavelength is less than 0.575
Calculated sin(theta_max)/wavelength = 0.5618

```
PLAT031_ALERT_4_B Refined Extinction Parameter Within Range ......      2.200 Sigma
PLAT084_ALERT_3_B High wR2 Value (i.e. > 0.25) ...................       0.36 Report
PLAT242_ALERT_2_B Low    'MainMol' Ueq as Compared to Neighbors of       C049 Check
PLAT242_ALERT_2_B Low    'MainMol' Ueq as Compared to Neighbors of       C05E Check
PLAT360_ALERT_2_B Short  C(sp3)-C(sp3) Bond  C053     - C05F     .       1.24 Ang.
PLAT416_ALERT_2_B Short Intra D-H..H-D       H00T     ..H013     .       1.70 Ang.
                                             x,y,z  =      1_555 Check
PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L=    0.562       2324 Report
PLAT934_ALERT_3_B Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..          3 Check
```

Alert level C

```
PLAT052_ALERT_1_C Info on Absorption Correction Method   Not Given     Please Do !
PLAT082_ALERT_2_C High R1 Value ................................       0.11 Report
PLAT213_ALERT_2_C Atom C12            has ADP max/min Ratio .....        3.3 prolat
PLAT213_ALERT_2_C Atom C48            has ADP max/min Ratio .....        3.4 prolat
PLAT213_ALERT_2_C Atom C05F           has ADP max/min Ratio .....        3.1 prolat
PLAT213_ALERT_2_C Atom C05Q           has ADP max/min Ratio .....        3.4 prolat
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range       5.6 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range       7.0 Ratio
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)  Fe02     --S03      .       5.5 s.u.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C05A Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C05C Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       O00X Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       O010 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C02N Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C040 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C04K Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C04W Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C054 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C05I Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of       C03F Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.1 Note
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.01318 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C04I     - C04M     .       1.38 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C05O     - C05Q     .       1.42 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C01J     - C021     .       1.53 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C02E     - C02R     .       1.53 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C02T     - C03L     .       1.53 Ang.
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PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C03D     - C041     .       1.55 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C03G     - C045     .       1.55 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact  H04A     ..H053     .       1.96 Ang.
                                                     x,y,z  =      1_555 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      7.632 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.623 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).         8 Note
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....        25 Note
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .         1 Check
PLAT977_ALERT_2_C Check Negative Difference Density on Hk               -0.39 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H0AB             -0.36 eA-3
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Alert level G

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ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
                not performed for this radiation type.
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        22 Note
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............         9 Report
PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka   0.81000 Ang.
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)      0.03 Degree
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records         1 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records        10 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records         4 Report
PLAT300_ALERT_4_G Atom Site Occupancy of C1         Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C2         Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C5         Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C056       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C05B       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C05K       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C05N       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C0AA       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1         Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2A        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2B        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2C        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H5A        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H5B        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H05L       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H05M       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H05V       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H05W       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H05X       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H8AA       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Hj         Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Hk         Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1BA       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H0AB       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H0AC       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H0AD       Constrained at       0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )         2% Note
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C01U     -C02U          0.15 Ang.
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C04D     -C04X          0.19 Ang.
PLAT343_ALERT_2_G Unusual sp3      Angle Range in Main Residue for       C053 Check
PLAT410_ALERT_2_G Short Intra H...H Contact  H02G     ..H05L     .       2.12 Ang.
                                                     x,y,z  =      1_555 Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........          ! Info
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........        353 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       1707 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed           ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...         14 Note
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PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........       3.8 Low
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......    Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         0 Info
PLAT984_ALERT_1_G The Cl-f'=    0.1831 Deviates from the B&C-Value    0.1809 Check
PLAT984_ALERT_1_G The Fe-f'=    0.3573 Deviates from the B&C-Value    0.3558 Check
PLAT984_ALERT_1_G The  S-f'=    0.1552 Deviates from the B&C-Value    0.1530 Check
PLAT985_ALERT_1_G The Cl-f"=    0.2090 Deviates from the B&C-Value    0.2068 Check
PLAT985_ALERT_1_G The Fe-f"=    1.0787 Deviates from the B&C-Value    1.0748 Check
PLAT985_ALERT_1_G The  S-f"=    0.1633 Deviates from the B&C-Value    0.1616 Check
```

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   6 ALERT level A = Most likely a serious problem - resolve or explain
   9 ALERT level B = A potentially serious problem, consider carefully
  37 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  54 ALERT level G = General information/check it is not something unexpected

  10 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  44 ALERT type 2 Indicator that the structure model may be wrong or deficient
  15 ALERT type 3 Indicator that the structure quality may be low
  35 ALERT type 4 Improvement, methodology, query or suggestion
   2 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

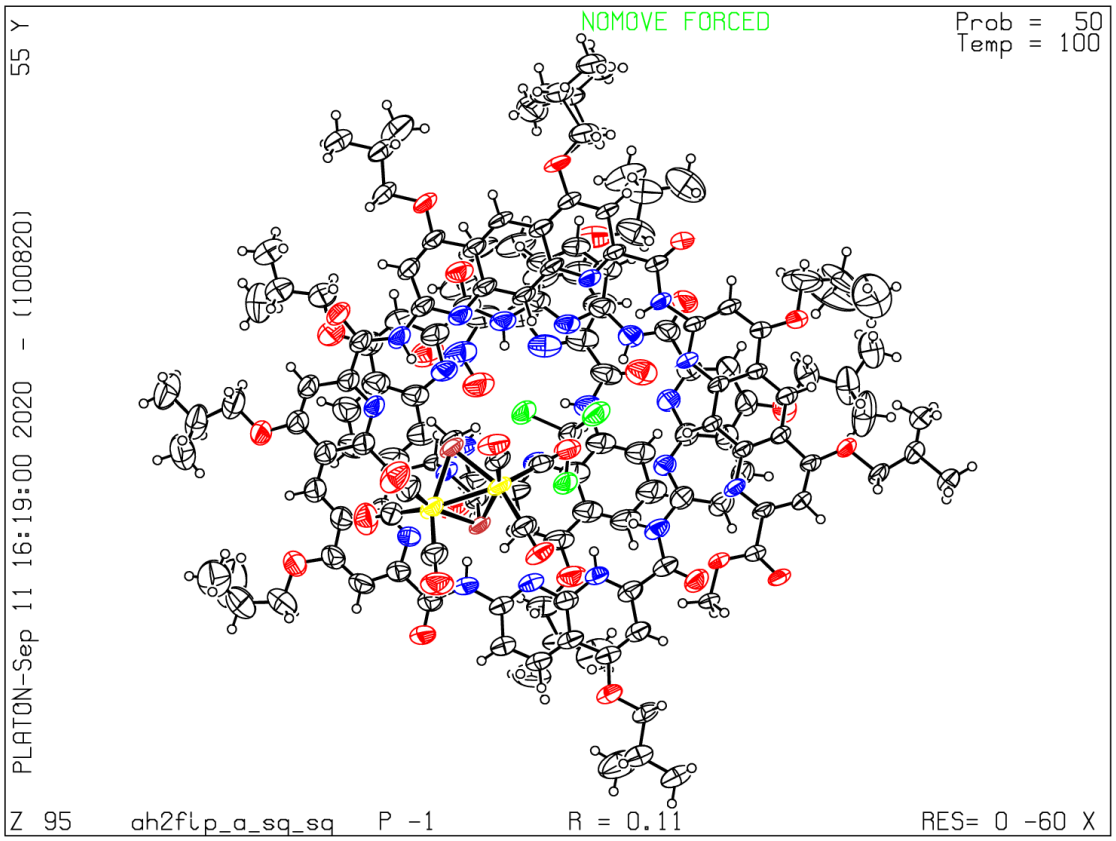
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 10/08/2020; check.def file version of 06/08/2020

Datablock ah2fip_a_sq_sq - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) squeezed

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: squeezed

Bond precision: C-C = 0.0232 A Wavelength=1.54178

Cell: a=26.6118(13) b=29.0835(13) c=36.1175(12)
alpha=83.259(3) beta=82.984(3) gamma=68.182(4)
Temperature: 100 K

	Calculated	Reported
Volume	25678(2)	25678(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C198 H204 Fe2 N30 O37 S2, 2(C H Cl3)	?
Sum formula	C200 H206 Cl6 Fe2 N30 O37 S2	C200 H206 Cl6 Fe2 N30 O37 S2
Mr	4010.48	4010.46
Dx,g cm-3	1.037	1.037
Z	4	4
Mu (mm-1)	2.149	2.149
F000	8392.0	8392.0
F000’	8418.56	
h,k,lmax	24,26,32	24,26,32
Nref	39970	35867
Tmin,Tmax	0.807,0.807	
Tmin’	0.807	

Correction method= Not given

Data completeness= 0.897 Theta(max)= 44.284

R(reflections)= 0.1170(9759) wR2(reflections)= 0.2564(35867)

S = 1.088 Npar= 4990

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level A

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
Calculated sin(theta_max)/wavelength = 0.4529
PLAT026_ALERT_3_A Ratio Observed / Unique Reflections (too) Low .. 27 %
PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low . 0.897 Note
PLAT602_ALERT_2_A VERY LARGE Solvent Accessible VOID(S) in Structure ! Info

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Alert level B

REFNR01_ALERT_3_B Ratio of reflections to parameters is < 8 for a
centrosymmetric structure
sine(theta)/lambda 0.4529
Proportion of unique data used 1.0000
Ratio reflections to parameters 7.1878
PLAT088_ALERT_3_B Poor Data / Parameter Ratio ..... 7.19 Note
PLAT220_ALERT_2_B Non-Solvent Resd 2 C Ueq(max)/Ueq(min) Range 6.1 Ratio
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of O31_13 Check
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C15_1 Check
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C33_1 Check
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of Cg_7 Check
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of O21_42 Check
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C22_31 Check
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C32_31 Check
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C33_31 Check
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C3_35 Check
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C23_45 Check
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C5_72 Check
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C_78 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of Ob_7 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of O_16 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of N_5 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of C22_1 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of Cd_7 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of C23_12 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of C33_12 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of C33_13 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of C22_15 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of O31_31 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of O8_72 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of N_35 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of C23_31 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of C16_33 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of Cd_37 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of C22_42 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of C11_42 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of C33_43 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of C23_44 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of C22_45 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of C33_45 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of C7_72 Check
PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.02318 Ang.
PLAT411_ALERT_2_B Short Inter H...H Contact H3_4 .. H1_87 . 1.86 Ang.
PLAT413_ALERT_2_B Short Inter XH3 .. XHn H18A_32.. H34B_42 .. 1.92 Ang.
PLAT911_ALERT_3_B Missing # FCF Refl Between THmin & STh/L= 0.453 4100 Report

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Alert level C

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PLAT052_ALERT_1_C Info on Absorption Correction Method   Not Given     Please Do !
PLAT082_ALERT_2_C High R1 Value ..................................      0.12 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ...................      0.26 Report
PLAT213_ALERT_2_C Atom C25_1           has ADP max/min Ratio .....       3.3 prolat
PLAT213_ALERT_2_C Atom C3_1            has ADP max/min Ratio .....       3.3 oblate
PLAT213_ALERT_2_C Atom C35_13          has ADP max/min Ratio .....       3.9 prolat
PLAT213_ALERT_2_C Atom C23_15          has ADP max/min Ratio .....       3.4 prolat
PLAT213_ALERT_2_C Atom O_54            has ADP max/min Ratio .....       3.6 prolat
PLAT213_ALERT_2_C Atom C25_31          has ADP max/min Ratio .....       3.1 prolat
PLAT213_ALERT_2_C Atom C22_31          has ADP max/min Ratio .....       3.5 prolat
PLAT213_ALERT_2_C Atom C33_31          has ADP max/min Ratio .....       3.5 prolat
PLAT213_ALERT_2_C Atom C24_44          has ADP max/min Ratio .....       3.7 prolat
PLAT213_ALERT_2_C Atom C23_45          has ADP max/min Ratio .....       3.3 oblate
PLAT213_ALERT_2_C Atom C35_45          has ADP max/min Ratio .....       3.1 oblate
PLAT213_ALERT_2_C Atom C9_72           has ADP max/min Ratio .....       3.5 prolat
PLAT214_ALERT_2_C Atom C1_85   (Anion/Solvent) ADP max/min Ratio         4.7 prolat
PLAT220_ALERT_2_C Non-Solvent Resd 1   C   Ueq(max)/Ueq(min) Range       5.4 Ratio
PLAT220_ALERT_2_C Non-Solvent Resd 2   O   Ueq(max)/Ueq(min) Range       3.1 Ratio
PLAT222_ALERT_3_C Non-Solvent Resd 1   H Uiso(max)/Uiso(min) Range       5.7 Ratio
PLAT222_ALERT_3_C Non-Solvent Resd 2   H Uiso(max)/Uiso(min) Range       7.6 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of     O21_1 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      Ob_5 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      Ob_6 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of    O21_13 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of     N63_1 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of     N0_15 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      C7_1 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      C6_1 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      C3_2 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      C8_2 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      C4_3 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      C3_4 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      C6_4 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      C5_5 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      C9_5 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      C3_6 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      C4_6 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      C4_7 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      C8_7 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of     C9_12 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of     C2_13 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of     C6_14 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of    C12_15 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of    C10_15 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of     C7_15 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of     C7_71 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of     Ob_35 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of     Ob_36 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of    O21_43 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of    O10_72 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of    N14_31 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of    N63_31 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of     N1_33 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      N_36 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of     N0_45 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of    C12_31 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of    C10_31 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of     C7_31 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of    C61_31 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of    C62_31 Check
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PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C3_32 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C6_32 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C6_33 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C15_33 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C3_34 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C5_34 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C10_35 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C4_36 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C2_37 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C4_37 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C10_37 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of Cg_37 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C12_42 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C15_42 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C8_42 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C4_42 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C32_42 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C1_43 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C22_44 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C1_44 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C11_45 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C2_72 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of S64_1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of O31_1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of O10_71 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N11_3 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N1_3 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N7_4 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N1_4 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N11_5 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N11_6 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N14_12 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N0_12 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N6_14 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C23_1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C10_1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C60_1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C16_2 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C4_2 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C5_2 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C9_2 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C3_3 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C5_4 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C8_5 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C_5 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Cd_5 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C2_6 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C5_7 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C7_7 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C9_7 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C_7 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C2_12 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C32_12 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C11_13 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C3_13 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C32_13 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C23_14 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C13_14 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C33_14 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C11_15 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C13_15 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C2_71 Check

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PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      C4_71 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C_74 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C_75 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C_76 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C_82 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of    Fe02_50 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of     S64_31 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of     S65_31 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of     O21_31 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of     O31_42 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       O_46 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      N7_33 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of     N11_35 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       N_37 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of     N14_43 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      N6_43 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      N0_43 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      N6_44 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of     C13_31 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      C9_31 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      C4_31 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      C1_31 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of     C60_31 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of     C16_32 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      C5_32 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of     C12_32 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of     C15_32 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      C8_33 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      C2_35 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      C8_35 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      C9_35 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C_35 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      C2_36 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      Cg_36 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      Cd_36 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      C3_37 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      C7_37 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      C9_37 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of     C13_42 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      C7_42 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of     C33_42 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of     C22_43 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      C2_43 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      C2_44 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of     C33_44 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of     C13_45 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      C1_45 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      C1_72 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      C4_72 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C_79 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C_80 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of      C1_85 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of      C1_86 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of      C1_87 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of      C1_88 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........       O4# Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........      O31# Check
PLAT361_ALERT_2_C Long   C(sp3)-C(sp3) Bond   C32_12 -   C33_12 ..      1.65 Ang.
PLAT361_ALERT_2_C Long   C(sp3)-C(sp3) Bond   C33_31 -   C35_31 ..      1.65 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact   H2_1   ..  H32A_1  .      1.93 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact   H9_5   ..  Hg2_5   .      1.96 Ang.
PLAT413_ALERT_2_C Short Inter XH3 .. XHn     Hd_6   ..  He2B_37 ..      2.05 Ang.
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PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......     41.226 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      8.793 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      4.011 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      2.223 Check
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .          2 Check
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.          0 Info
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        564 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...        554 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............         18 Report
PLAT013_ALERT_1_G N.O.K. _shelx_hkl_checksum found in CIF ........     Please Check
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records        239 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records        211 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records        141 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records          1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          8 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records          1 Report
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C_73 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C_74 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C_81 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C_77 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C_78 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C_79 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C_84 Check
PLAT398_ALERT_2_G Deviating  C-O-C  Angle from 120 Deg for Ob_6        105.5 Degree
PLAT432_ALERT_2_G Short Inter X...Y Contact  O_37   ..  C1_88   ..      3.00 Ang.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........        966 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          5 Note
             C H Cl3
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       8374 Note
PLAT908_ALERT_2_G Max. Perc. Data with I > 2*s(I) per Res.Shell .      66.20% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          2 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          1 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...        104 Note
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......     Please Check
```

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   4 ALERT level A = Most likely a serious problem - resolve or explain
  41 ALERT level B = A potentially serious problem, consider carefully
 190 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  27 ALERT level G = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 228 ALERT type 2 Indicator that the structure model may be wrong or deficient
  18 ALERT type 3 Indicator that the structure quality may be low
  12 ALERT type 4 Improvement, methodology, query or suggestion
   2 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

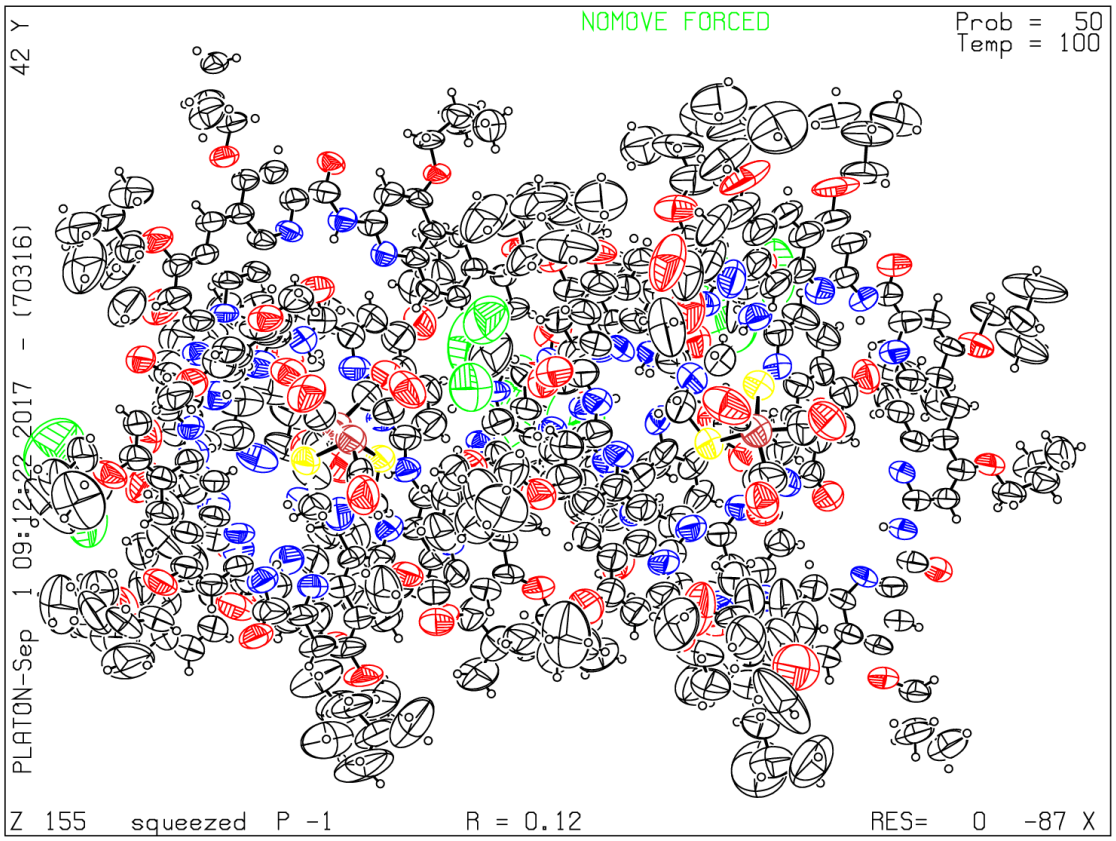
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 13/08/2017; check.def file version of 27/07/2017

Datablock squeezed - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) end_a

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: end_a

Bond precision: C-C = 0.0211 A Wavelength=1.54178

Cell: a=17.496(4) b=21.656(4) c=33.846(7)
alpha=97.71(3) beta=104.52(3) gamma=97.62(3)
Temperature: 130 K

	Calculated	Reported
Volume	12116(5)	12116(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C189 H193 Fe2 N30 O35 S2, C6 H5 Cl [+ solvent]	C189 H193 Fe2 N30 O35 S2, C6 H5 Cl
Sum formula	C195 H198 Cl Fe2 N30 O35 S2 [+ solvent]	C195 H198 Cl Fe2 N30 O35 S2
Mr	3733.12	3733.09
Dx,g cm-3	1.023	1.023
Z	2	2
Mu (mm-1)	1.744	1.744
F000	3918.0	3918.0
F000’	3927.23	
h,k,lmax	15,19,30	15,19,30
Nref	19054	18810
Tmin,Tmax	0.840,0.840	
Tmin’	0.840	

Correction method= Not given

Data completeness= 0.987 Theta(max)= 44.491

R(reflections)= 0.0890(7894) wR2(reflections)= 0.2566(18810)

S = 0.873 Npar= 2417

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level A

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
Calculated sin(theta_max)/wavelength = 0.4545
PLAT213_ALERT_2_A Atom C047 has ADP max/min Ratio ..... 5.1 oblate
PLAT234_ALERT_4_A Large Hirshfeld Difference C04X --C061 . 0.32 Ang.
PLAT241_ALERT_2_A High 'MainMol' Ueq as Compared to Neighbors of C07D Check
PLAT360_ALERT_2_A Short C(sp3)-C(sp3) Bond C05U - C07D . 1.22 Ang.
PLAT362_ALERT_2_A Short C(sp3)-C(sp2) Bond C06X - C07F . 1.14 Ang.
PLAT410_ALERT_2_A Short Intra H...H Contact H04G ..H05X . 1.69 Ang.
x,y,z = 1_555 Check

Alert level B

PLAT088_ALERT_3_B Poor Data / Parameter Ratio ..... 7.78 Note
PLAT230_ALERT_2_B Hirshfeld Test Diff for N00R --C03E . 7.5 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for N023 --C03C . 7.5 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for C031 --C034 . 7.3 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for C039 --C05F . 7.6 s.u.
PLAT234_ALERT_4_B Large Hirshfeld Difference O01X --N01I . 0.27 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference C022 --C04Q . 0.28 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference C03H --C05C . 0.28 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference C03I --C04N . 0.28 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference C047 --C04T . 0.27 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference C04N --C04X . 0.27 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference C04S --C05E . 0.27 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference C052 --C05V . 0.26 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference C05L --C06K . 0.28 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference C05Y --C06I . 0.28 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference C065 --C077 . 0.26 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference Cl00 --C06P . 0.28 Ang.
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C06X Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of C05U Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of C05Z Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of C081 Check
PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.02108 Ang.
PLAT360_ALERT_2_B Short C(sp3)-C(sp3) Bond C16 - C075 . 1.29 Ang.
PLAT360_ALERT_2_B Short C(sp3)-C(sp3) Bond C06A - C078 . 1.31 Ang.
PLAT410_ALERT_2_B Short Intra H...H Contact H05X ..H07M . 1.80 Ang.
x,y,z = 1_555 Check
PLAT412_ALERT_2_B Short Intra XH3 .. XHn H06F ..H0AD . 1.77 Ang.
x,y,z = 1_555 Check

Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.143
PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 ..... 0.143 Report
PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low .. 42% Check
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..... 0.26 Report
PLAT213_ALERT_2_C Atom C16 has ADP max/min Ratio ..... 3.8 prolat
PLAT213_ALERT_2_C Atom C18 has ADP max/min Ratio ..... 3.7 prolat
PLAT213_ALERT_2_C Atom C03Y has ADP max/min Ratio ..... 3.3 prolat
PLAT213_ALERT_2_C Atom C063 has ADP max/min Ratio ..... 3.3 prolat
PLAT213_ALERT_2_C Atom C06X has ADP max/min Ratio ..... 3.5 prolat
PLAT213_ALERT_2_C Atom C073 has ADP max/min Ratio ..... 3.1 prolat
PLAT213_ALERT_2_C Atom C07D has ADP max/min Ratio ..... 3.2 prolat

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PLAT213_ALERT_2_C Atom C07V           has ADP max/min Ratio .....       4.0 prolat
PLAT213_ALERT_2_C Atom C0AA           has ADP max/min Ratio .....       3.3 prolat
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range       6.0 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range       7.0 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for    O00O     --C046     .       5.5 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    N00Q     --C02M     .       6.8 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    N00U     --C02J     .       6.3 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    N01V     --C05D     .       6.9 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C02R     --C03H     .       6.8 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C02V     --C03B     .       6.8 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C037     --C04T     .       6.8 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C043     --C04E     .       6.1 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C046     --C04O     .       5.4 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C047     --C05J     .       5.5 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C04O     --C05C     .       5.2 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C04Y     --C056     .       6.3 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C051     --C070     .       5.1 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C052     --C064     .       6.1 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference Fe01     --C05I     .      0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O005     --C04M     .      0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O007     --C02M     .      0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O008     --C03Q     .      0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O00E     --C05Y     .      0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O00W     --C05A     .      0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O016     --C03P     .      0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O016     --C05Z     .      0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O018     --C05M     .      0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O019     --C064     .      0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O01D     --C04Z     .      0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O01Z     --C05I     .      0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O027     --C046     .      0.23 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O02K     --C03Y     .      0.25 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N00A     --C020     .      0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N00A     --C025     .      0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N00I     --C028     .      0.25 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N00M     --C03K     .      0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N00M     --C049     .      0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N00Q     --C020     .      0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N00T     --C02V     .      0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N00V     --C02O     .      0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N012     --C025     .      0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N012     --C03G     .      0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N01A     --C038     .      0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N01B     --C03U     .      0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N01F     --C044     .      0.24 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N01J     --C04B     .      0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N01O     --C03A     .      0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N01V     --C05Q     .      0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N01W     --C02Y     .      0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N01Y     --C05B     .      0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C01P     --C02L     .      0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C01P     --C041     .      0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C01R     --C033     .      0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C01T     --C021     .      0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C020     --C04E     .      0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C024     --C03F     .      0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C026     --C04G     .      0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C02A     --C04H     .      0.24 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C02B     --C02T     .      0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C02C     --C045     .      0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C02F     --C03T     .      0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C02H     --C032     .      0.17 Ang.
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PLAT234_ALERT_4_C Large Hirshfeld Difference C02I --C03S . 0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C02N --C02X . 0.23 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C02P --C035 . 0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C02Q --C050 . 0.25 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C02S --C03N . 0.23 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C02U --C04U . 0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C02W --C03F . 0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C02W --C04D . 0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C02Z --C030 . 0.23 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C038 --C04L . 0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C039 --C03B . 0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C03B --C03O . 0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C03D --C03P . 0.24 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C03D --C03V . 0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C03J --C053 . 0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C03M --C04H . 0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C03N --C03T . 0.24 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C03Q --C060 . 0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C03V --C040 . 0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C04A --C04Q . 0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C04A --C04W . 0.24 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C04D --C04F . 0.25 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C04M --C05P . 0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C04Q --C05W . 0.25 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C04U --C05G . 0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C04V --C05O . 0.25 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C04W --C05X . 0.24 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C04Y --C05B . 0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C04Z --C05J . 0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C051 --C054 . 0.23 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C05N --C05P . 0.24 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C05T --C05W . 0.23 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C060 --C06Q . 0.20 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O00Y Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of N01W Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C045 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C04C Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C04E Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C04L Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C04M Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C04N Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C04U Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C05I Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C061 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C063 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C064 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C06L Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Fe01 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Fe02 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of O00O Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of O00X Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of O019 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C022 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C16 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C02Y Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C03C Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C03I Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C03O Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C03Q Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C04J Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C04P Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C04X Check

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PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C04Y Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C04Z Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C051 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C05L Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C05P Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C05R Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C065 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C066 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C06C Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C06I Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C073 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C078 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of       C06P Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.9 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      Fe01      0.128 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      Cl00      0.208 Check
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C2       - C066     .       1.41 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C06I     - C07L     .       1.43 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C073     - C07V     .       1.36 Ang.
PLAT361_ALERT_2_C Long   C(sp3)-C(sp3) Bond  C16      - C067     .       1.71 Ang.
PLAT361_ALERT_2_C Long   C(sp3)-C(sp3) Bond  C078     - C07Q     .       1.70 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C038     - C049     .       1.53 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C04Z     - C05J     .       1.53 Ang.
PLAT412_ALERT_2_C Short Intra XH3 .. XHn     H07D     ..H0AC     .       1.85 Ang.
                                                    x,y,z  =      1_555 Check
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...     -6.206 Report
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.455        244 Report
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          8 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         47 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............         10 Report
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.15 Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)       0.03 Degree
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          4 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records         12 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Fe01     --C03Y     .        7.2 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Fe02     --S003     .        7.7 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Fe02     --C063     .        6.2 s.u.
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C063 Check
PLAT343_ALERT_2_G Unusual sp3      Angle Range in Main Residue for       C07D Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C02Z     ..C04N            3.20 Ang.
                                                  1+x,y,z  =      1_655 Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........          ! Info
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........        444 Note
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C067     --C16            1.71 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C078     --C07Q           1.70 Ang.
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        231 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed          ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          2 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          1 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          8 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        4.2 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          1 Info
```

```
  7 ALERT level A = Most likely a serious problem - resolve or explain
 26 ALERT level B = A potentially serious problem, consider carefully
161 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 25 ALERT level G = General information/check it is not something unexpected
```

```
  2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
106 ALERT type 2 Indicator that the structure model may be wrong or deficient
 14 ALERT type 3 Indicator that the structure quality may be low
 96 ALERT type 4 Improvement, methodology, query or suggestion
  1 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

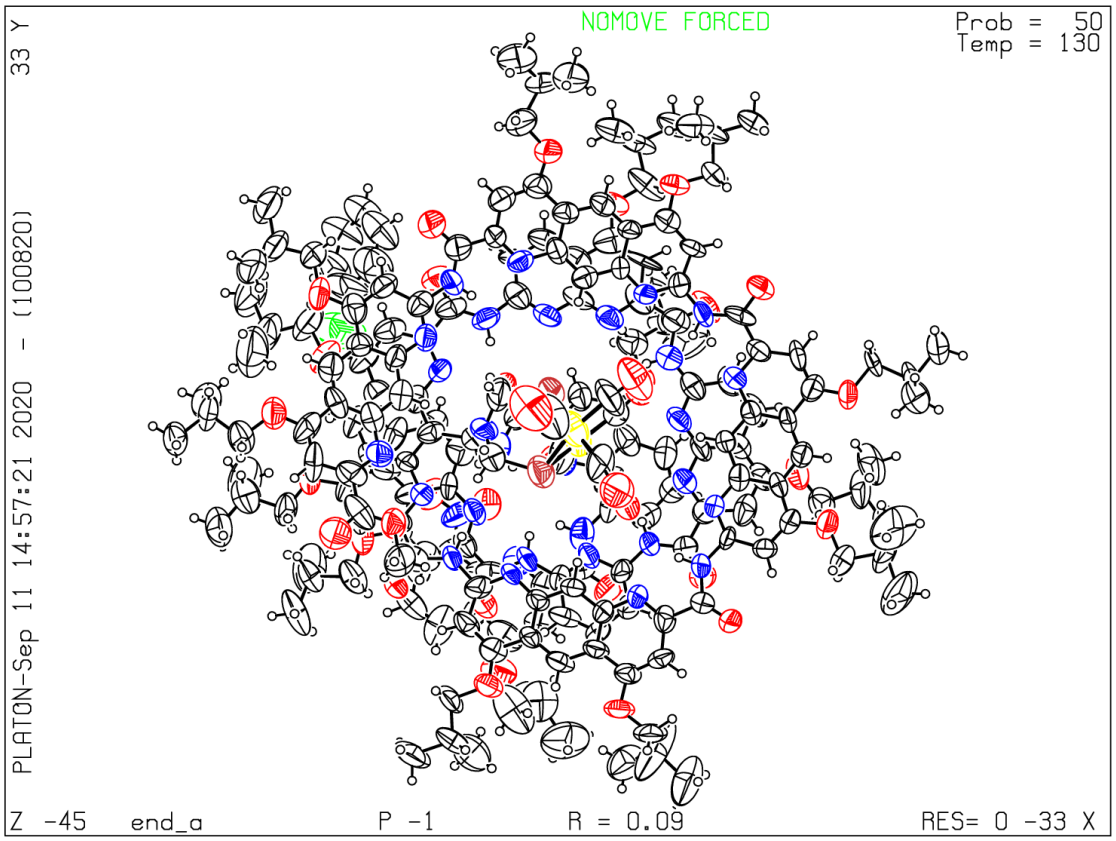
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 10/08/2020; check.def file version of 06/08/2020

Datablock end_a - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) a-fe_fip2011

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: a-fe_fip2011

```
Bond precision:  C-C = 0.0083 A          Wavelength=0.80000

Cell:          a=11.614(2)      b=11.913(2)      c=14.995(3)
               alpha=90.34(3)   beta=100.67(3)   gamma=114.20(3)
Temperature:   100 K
```

	Calculated	Reported
Volume	1851.9(8)	1851.9(8)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C33 H33 Fe2 N3 O12 S2	C33 H33 Fe2 N3 O12 S2
Sum formula	C33 H33 Fe2 N3 O12 S2	C33 H33 Fe2 N3 O12 S2
Mr	839.44	839.44
Dx,g cm-3	1.505	1.505
Z	2	2
Mu (mm-1)	1.320	1.329
F000	864.0	864.0
F000’	866.58	
h,k,lmax	12,12,15	12,12,15
Nref	4528	3993
Tmin,Tmax		
Tmin’		

```
Correction method= Not given

Data completeness= 0.882          Theta(max)= 24.895

R(reflections)= 0.0575( 3617)     wR2(reflections)= 0.1550( 3993)

S = 1.038                 Npar= 507
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level A

```
THETM01_ALERT_3_A  The value of sine(theta_max)/wavelength is less than 0.550
           Calculated sin(theta_max)/wavelength =    0.5262
PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low .      0.882 Why?
```

Alert level B

```
PLAT088_ALERT_3_B Poor Data / Parameter Ratio ...................       7.88 Note
PLAT213_ALERT_2_B Atom C17A           has ADP max/min Ratio .....        4.7 oblate
PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L=    0.526        533 Report
```

Alert level C

```
PLAT213_ALERT_2_C Atom O5             has ADP max/min Ratio .....        3.1 oblate
PLAT213_ALERT_2_C Atom C20B           has ADP max/min Ratio .....        3.4 prolat
PLAT213_ALERT_2_C Atom C201           has ADP max/min Ratio .....        3.3 oblate
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range       4.3 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range       4.3 Ratio
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....       2.4 Note
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00828 Ang.
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....         4 Note
PLAT977_ALERT_2_C Check Negative Difference Density on H28A            -0.32 eA-3
```

Alert level G

```
ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
               not performed for this radiation type.
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          6 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large       6.58 Why ?
PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka    0.80000 Ang.
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)       0.03 Degree
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          1 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records          1 Report
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )         8% Note
PLAT432_ALERT_2_G Short Inter X...Y Contact  O605     ..C202           2.90 Ang.
                                              2-x,2-y,-z  =      2_775 Check
PLAT722_ALERT_1_G Angle   Calc      110.00, Rep      108.90 Dev...       1.10 Degree
             H17A    -C17A    -H17B       1.555  1.555  1.555     #  151 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        465 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        82% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          2 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...         20 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        2.8 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          1 Info
PLAT984_ALERT_1_G The Fe-f'=    0.3685 Deviates from the B&C-Value     0.3563 Check
PLAT985_ALERT_1_G The Fe-f"=    1.0547 Deviates from the B&C-Value     1.0512 Check
```

```
   2 ALERT level A = Most likely a serious problem - resolve or explain
   3 ALERT level B = A potentially serious problem, consider carefully
   9 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  19 ALERT level G = General information/check it is not something unexpected

   6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
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  12 ALERT type 3 Indicator that the structure quality may be low
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   0 ALERT type 5 Informative message, check
```

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Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 26/06/2020; check.def file version of 17/06/2020

Datablock a-fe_fip2011 - ellipsoid plot